

=> d ibib abs hitstr 1

L13 ANSWER 1 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:893130 HCAPLUS

DOCUMENT NUMBER: 134:222969

TITLE: Synthesis and characterization of a tetranucleotide analog containing alternating phosphonate-amide backbone linkages

AUTHOR(S): Yu, P.; Wang, W.; Zhang, H.; Yang, X.; Liang, T. C.; Gao, X.

CORPORATE SOURCE: Department of Chemistry, University of Houston, Houston, TX, 77204-5641, USA

SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(1), 107-119
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:222969

AB Described herein is the synthesis and characterization of a tetranucleotide, 5'-dC-phosphonate-T-amide-T-phosphonate-dC (III), in which the C-T and T-C steps contain a phosphonate backbone bond and T-T is a peptide nucleic acid dimer unit (neutral backbone). The 5'- and 3'-OH groups of the tetramer can be further derivatized and, thus, the compd. is a potential building block for longer oligonucleotides which will contain alternating backbone modifications at designated positions. The synthesis involved first the prepn. of two hybrid peptide-deoxyribose dinucleotides, CT-CO (I) and N-CT (II) (C and T are nucleobases; CO and N are carboxylic and amino terminal, resp.); each is linked through a phosphonate linkage. A condensation reaction between the two dimers, followed by deprotection, resulted in the formation of a peptide linkage to give the desired tetramer III. The reaction conditions used are mild to afford products in moderate to excellent yields. The DNA-PNA-DNA tetramer, d(CTTC), is a substrate for T4 kinase but fails to give a ligation product, even though NMR shows weak interactions between the tetramer III with its complementary sequence, d(GAAG).

IT 329326-31-0P

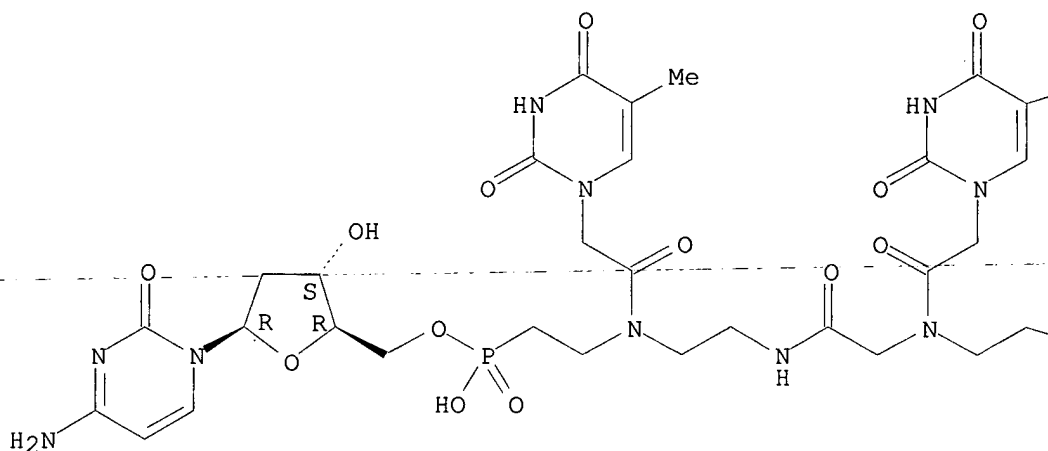
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(synthesis and characterization of a tetranucleotide analog contg. alternating phosphonate-amide backbone linkages as enzyme substrates)

RN 329326-31-0 HCAPLUS

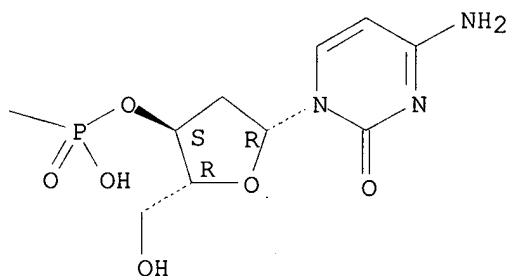
CN Cytidine, 2'-deoxycytidylyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino] (2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



IT 329326-42-3P 329326-43-4P 329326-44-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

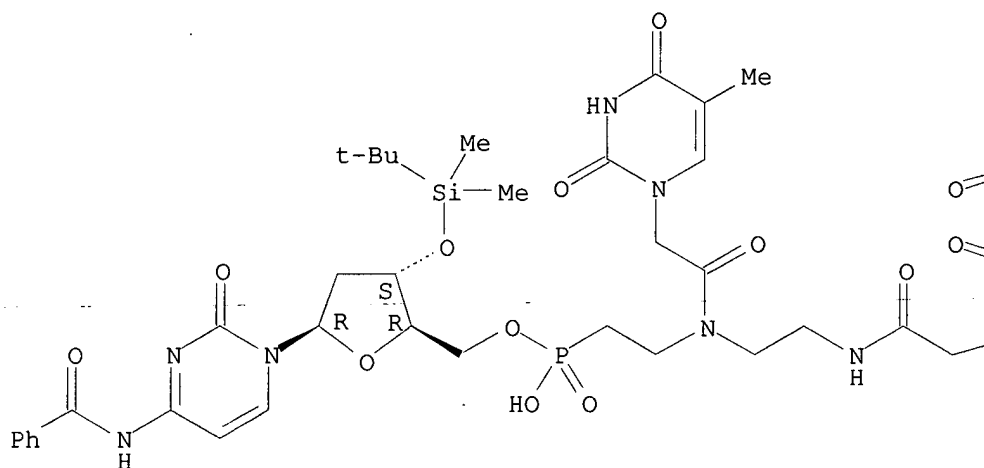
(synthesis and characterization of a tetranucleotide analog contg.
alternating phosphonate-amide backbone linkages as enzyme substrates)

RN 329326-42-3 HCAPLUS

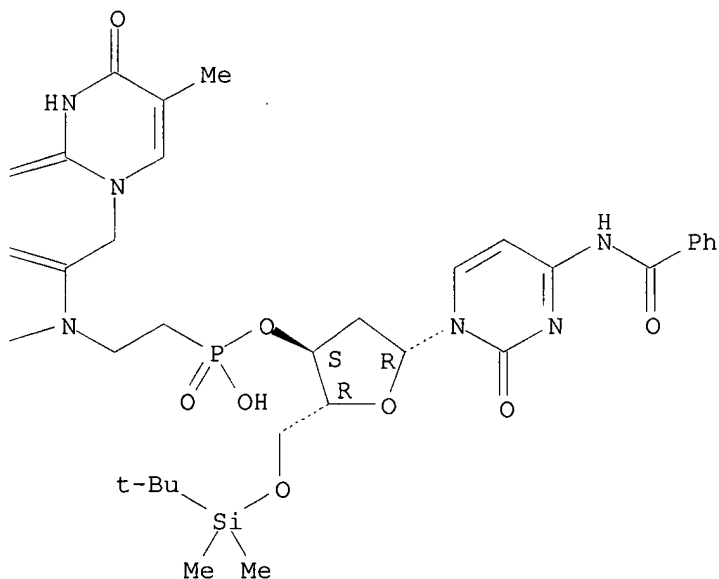
CN Cytidine, N-benzoyl-2'-deoxy-5'-O-[(1,1-dimethylethyl)dimethylsilyl]cytidyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino] (2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-N-benzoyl-2'-deoxy-3'-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

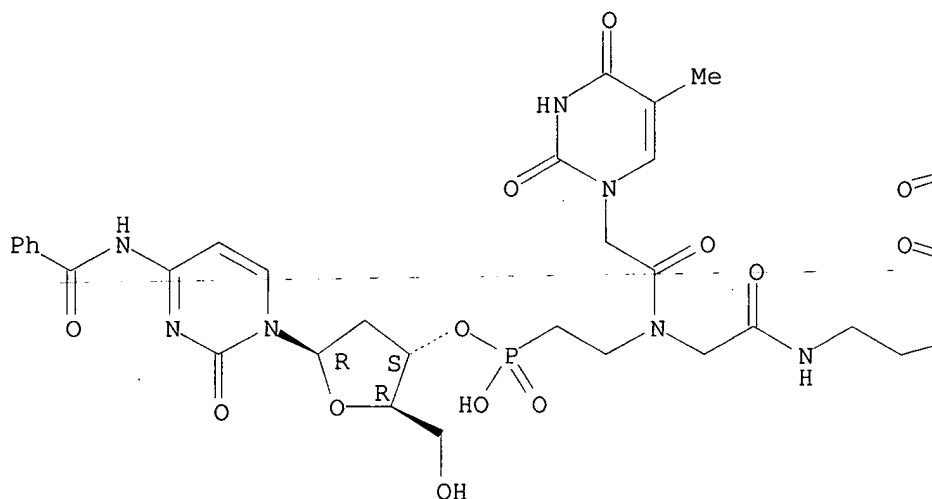


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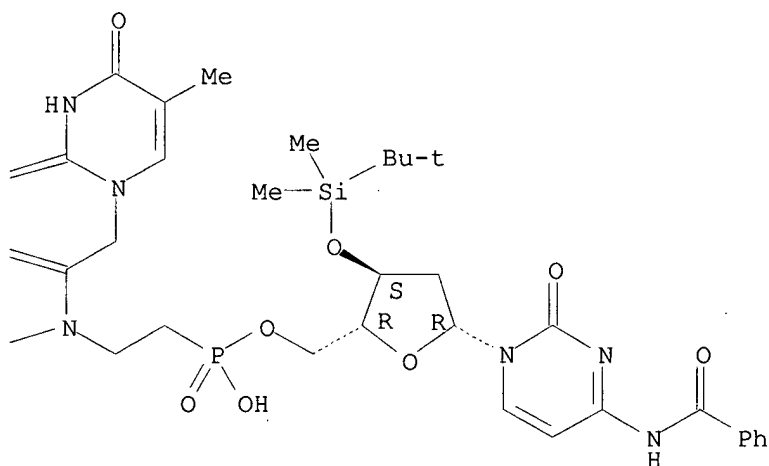
CN Cytidine, N-benzoyl-2'-deoxycytidylyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino] (2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-N-benzoyl-2'-deoxy-3'-O-[(1,1-dimethylethyl)dimethylsilyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

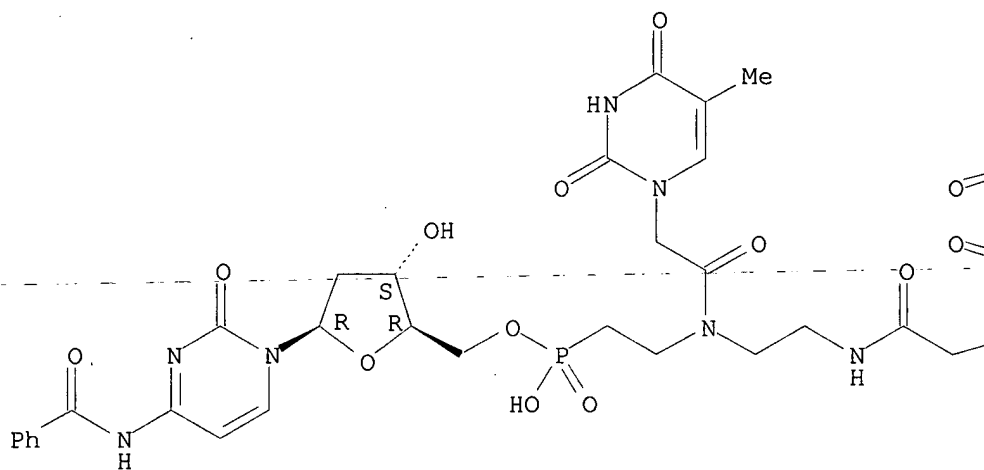


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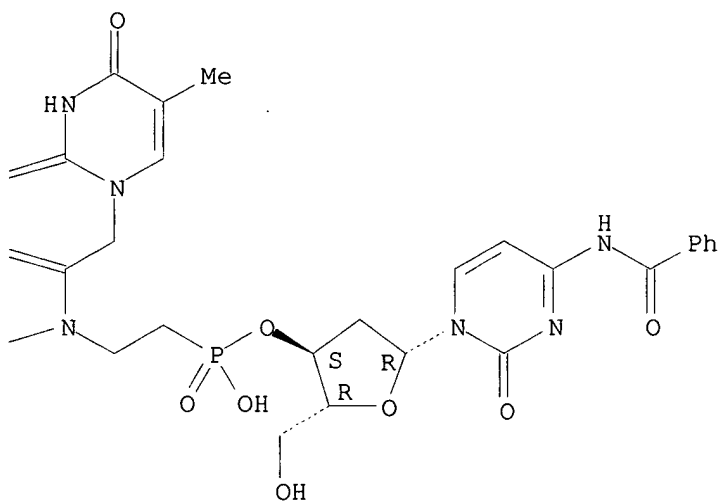
CN Cytidine, N-benzoyl-2'-deoxycytidylyl-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino] (2-oxo-1,2-ethanediyl)imino-1,2-ethanediyl[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]imino]-1,2-ethanediylphosphinico-(3'.fwdarw.5')-N-benzoyl-2'-deoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B



REFERENCE COUNT:

49

THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 2

L13 ANSWER 2 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:458348 HCAPLUS

DOCUMENT NUMBER: 133:238287

TITLE: Convergent synthesis of ribonuclease L-active
2',5'-oligoadenylate-peptide nucleic acids

AUTHOR(S): Wang, Zhengfu; Chen, Ling; Bayly, Suzanne F.;
Torrence, Paul F.

CORPORATE SOURCE: Section on Biomedical Chemistry, Laboratory of
Medicinal Chemistry, National Institute of Diabetes
and Digestive and Kidney Diseases, National Institutes
of Health, Bethesda, MD, 20892-0805, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2000),
10(12), 1357-1360

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB 2-5A [(p5'A2')np5'A] was conjugated to N-(2-aminoethyl)-glycyl PNA by
periodate oxidn., followed by coupling with amino-derivatized PNA and
final cyanoborohydride redn. An adduct of 2-5A pentamer with tetrameric
thymine PNA activated RNase L with the same potency as earlier versions of
2-5A-PNA or 2-5A-DNA.

IT **292609-04-2P 292609-05-3P**

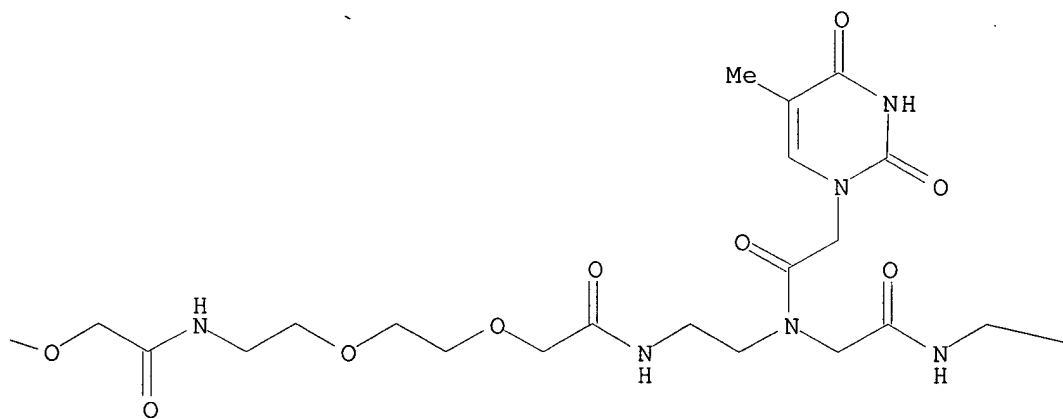
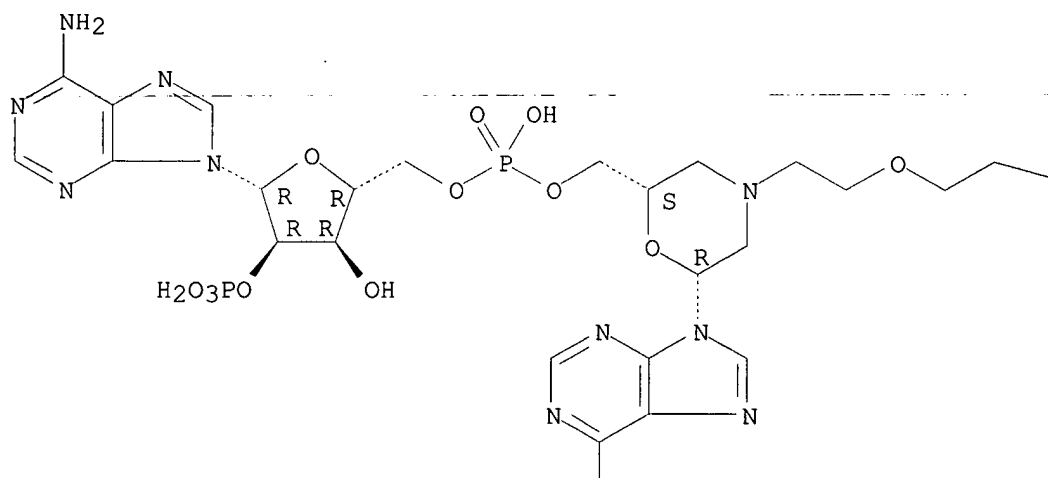
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)

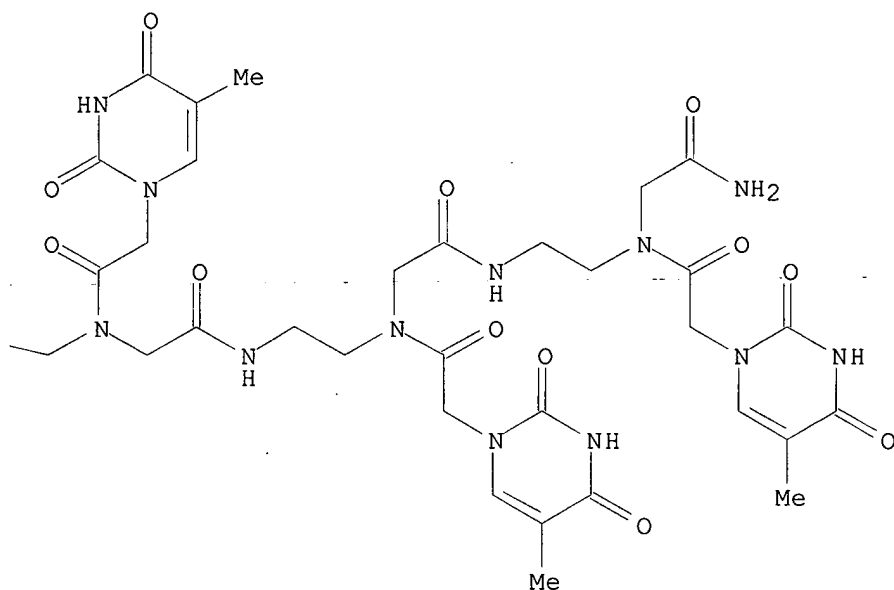
(convergent synthesis of RNase L-active oligoadenylate-peptide nucleic
acids)

RN 292609-04-2 HCAPLUS

CN 2'-Adenylic acid, 5'-[[(2S,6R)-6-(6-amino-9H-purin-9-yl)-4-[41-amino-
21,27,33,39-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-
pyrimidinyl)acetyl]-8,17,23,29,35,41-hexaoxo-3,6,12,15-tetraoxa-
9,18,21,24,27,30,33,36,39-nonaazahentetracont-1-yl]-2-morpholinyl]methyl
hydrogen phosphate] (9CI) (CA INDEX NAME)

Absolute stereochemistry.



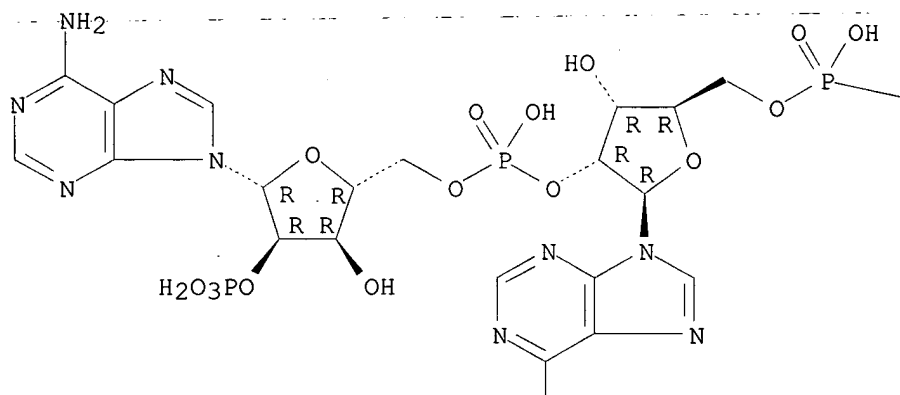


RN 292609-05-3 HCAPLUS

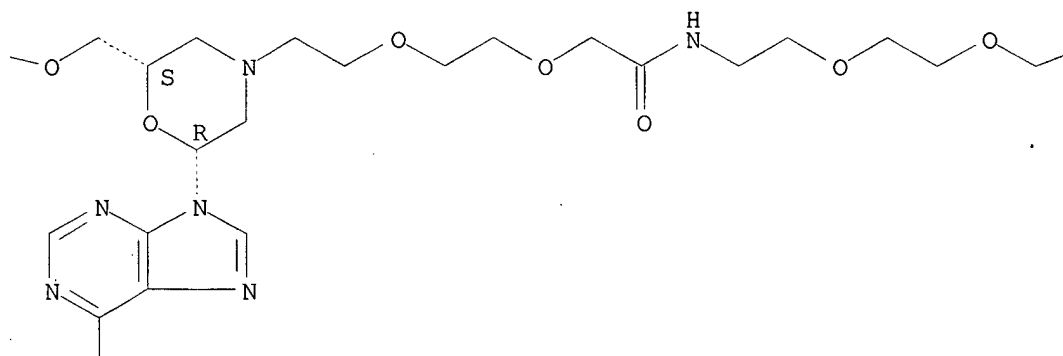
CN 2'-Adenylic acid, 5'-O-[[[(2S,6R)-6-(6-amino-9H-purin-9-yl)-4-[41-amino-21,27,33,39-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8,17,23,29,35,41-hexaoxo-3,6,12,15-tetraoxa-9,18,21,24,27,30,33,36,39-nonaazahentetracont-1-yl]-2-morpholinyl]methoxy]hydroxyphosphinyl]adenyl-yl-(2'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

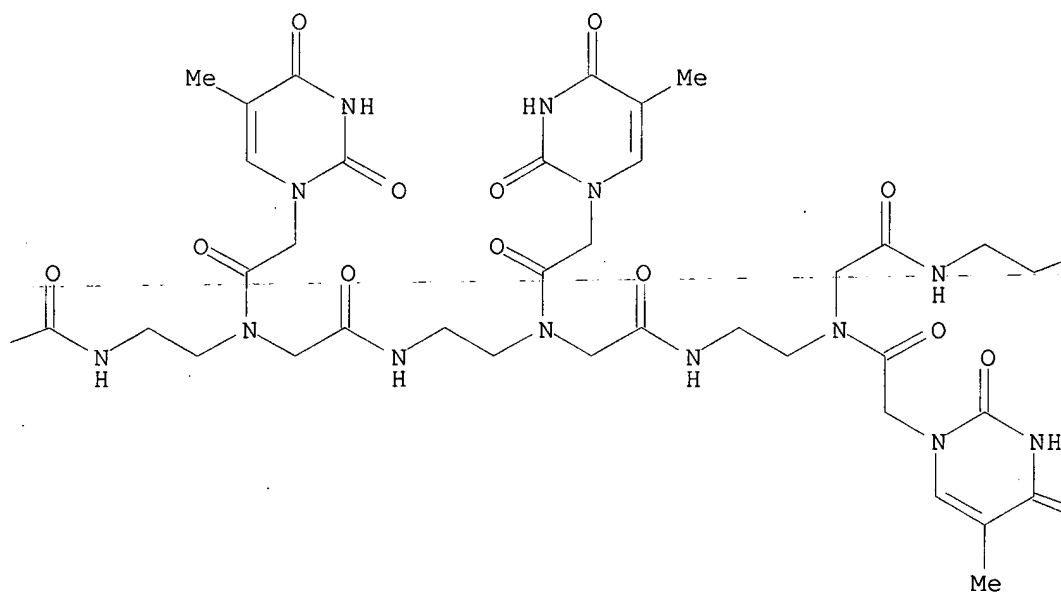
PAGE 1-A



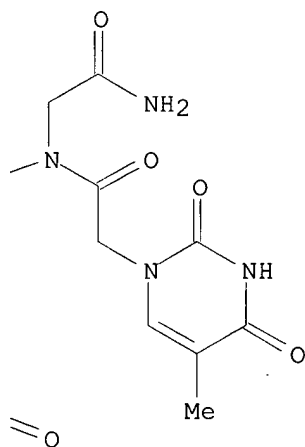
PAGE 1-B



PAGE 1-C



PAGE 1-D



PAGE 2-A



NH₂

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 3

L13 ANSWER 3 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2000:89855 HCAPLUS

DOCUMENT NUMBER: 132:245836

TITLE: Acyclic Analogues of Deoxyadenosine
3',5'-Bisphosphates as P2Y1 Receptor AntagonistsAUTHOR(S): Kim, Yong-Chul; Gallo-Rodriguez, Carola; Jang,
Soo-Yeon; Nandan, Erathodiyil; Adams, Mary; Harden,
T. Kendall; Boyer, Jose L.; Jacobson, Kenneth A.CORPORATE SOURCE: Molecular Recognition Section Laboratory of Bioorganic
Chemistry National Institute of Diabetes Digestive and
Kidney Diseases, National Institutes of Health,
Bethesda, MD, 20892-0810, USASOURCE: Journal of Medicinal Chemistry (2000), 43(4), 746-755
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB P2Y1 receptors are activated by ADP and occur on endothelial cells, smooth muscle, epithelial cells, lungs, pancreas, platelets, and in the central nervous system. With the aid of mol. modeling, we have designed nucleotide analogs that act as selective antagonists at this subtype. The present study has tested the hypothesis that acyclic modifications of the ribose ring, proven highly successful for nucleoside antiviral agents such as gancyclovir, are generalizable to P2Y receptor ligands. Specifically, the binding site of the P2Y1 receptor was found to be sufficiently accommodating to allow the substitution of the ribose group with acyclic aliph. and arom. chains attached to the 9-position of adenine. Three groups of adenine derivs. having diverse side-chain structures, each contg. two sym. phosphate or phosphonate groups, were prep. Biol. activity was demonstrated by the ability of the acyclic derivs. to act as agonists or antagonists in the stimulation of phospholipase C in turkey erythrocyte membranes. An acyclic N6-methyladenine deriv., 2-[2-(6-methylamino-purin-9-yl)-ethyl]-propane-1,3-bisoxo(diammoniumphosphate) (10), contg. an isopentyl bisphosphate moiety, was a full antagonist at the P2Y1 receptor with an IC50 value of 1.60 .mu.M. The corresponding 2-Cl deriv. (11) was even more potent with an IC50 value of 0.84 .mu.M. Homologation of the ethylene group at the 9-position to 3-5 methylene units or inclusion of cis- or trans-olefinic groups greatly reduced antagonist potency at the P2Y1 receptor. Analogs contg. a diethanolamine amide group and an aryl di(methylphosphonate) were both less potent than 10 as antagonists, with IC50 values of 14 and 16 .mu.M, resp., and no agonist activity was obsd. for these analogs. Thus, the ribose moiety is clearly not essential for recognition by the turkey P2Y1 receptor, although a cyclic structure appears to be important for receptor activation, and the acyclic approach to the design of P2 receptor antagonists is valid.

IT 262863-42-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(acyclic analogs of deoxyadenosine 3',5'-bisphosphates as P2Y1 receptor antagonists)

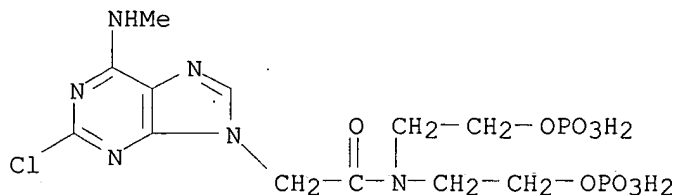
RN 262863-42-3 HCAPLUS

CN 9H-Purine-9-acetamide, 2-chloro-6-(methylamino)-N,N-bis[2-(phosphonooxy)ethyl]-, compd. with N,N-diethylethanamine (1:1), triammonium salt (9CI) (CA INDEX NAME)

CM 1

CRN 262863-41-2

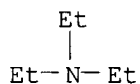
CMF C12 H19 Cl N6 O9 P2



CM 2

CRN 121-44-8

CMF C6 H15 N



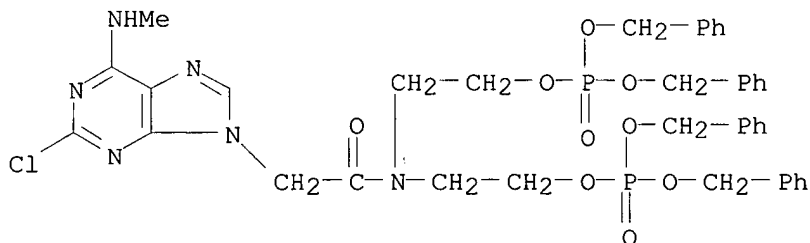
IT 262863-49-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(acyclic analogs of deoxyadenosine 3',5'-bisphosphates as P2Y1 receptor antagonists)

RN 262863-49-0 HCAPLUS

CN Phosphoric acid, [[[2-chloro-6-(methylamino)-9H-purin-9-yl]acetyl]imino]di-2,1-ethanediyl tetrakis(phenylmethyl) ester (9CI) (CA INDEX NAME)



REFERENCE COUNT:

30

THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 4

L13 ANSWER 4 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:290595 HCAPLUS

DOCUMENT NUMBER: 131:59111

TITLE: Peptide nucleic acids and their phosphonate analogues: synthesis and hybridization properties

AUTHOR(S): Efimov, V. A.; Buryakova, A. A.; Choob, M. V.; Chakhmakhlcheva, G.

CORPORATE SOURCE: Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Moscow, 117871, Russia

SOURCE: Bioorganicheskaya Khimiya (1998), 24(9), 696-709
CODEN: BIKHD7; ISSN: 0132-3423

PUBLISHER: MAIK Nauka

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The synthesis of a series of DNA mimics (peptide nucleic acids, phosphonate analogs of peptide nucleic acids, and their hybrids) is described. The preparative synthesis of the corresponding monomers and the solid phase automated synthesis of oligomers-mimics are developed. Modified phosphonate analogs of peptide nucleic acids, in particular chiral derivs. and those with addnl. hydroxyl groups in the side chains of the backbone as well as pyrene derivs. of peptide nucleic acids and their phosphonate analogs, are prepd. The ability of the resulting oligomers specifically to hybridize to DNA and RNA complementary chains is studied. It is shown that phosphonate analogs of peptide nucleic acids and their hybrids with peptide nucleic acids can form complexes with the DNA and RNA complementary strands, the stability of the complexes increasing in parallel with the increase in the no. of peptide nucleic acid residues in the chain of the mimic. This property, along with good water soly., provides the precondition for further evaluation of these compds. as antisense and antigene agents.

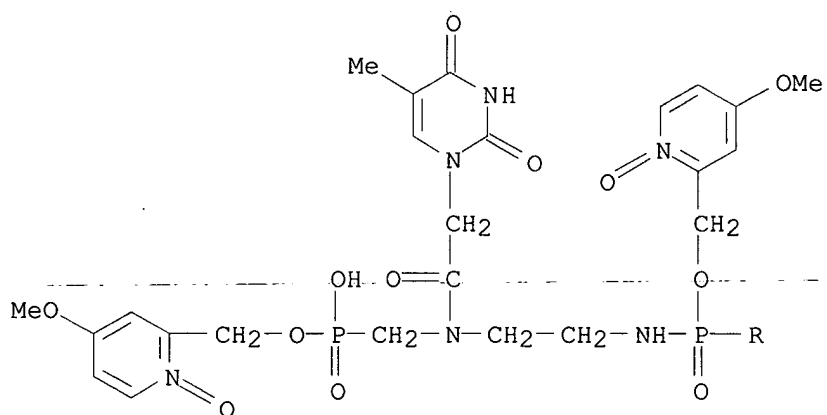
IT 227798-10-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and hybridization properties of peptide nucleic acids and their phosphonate analogs)

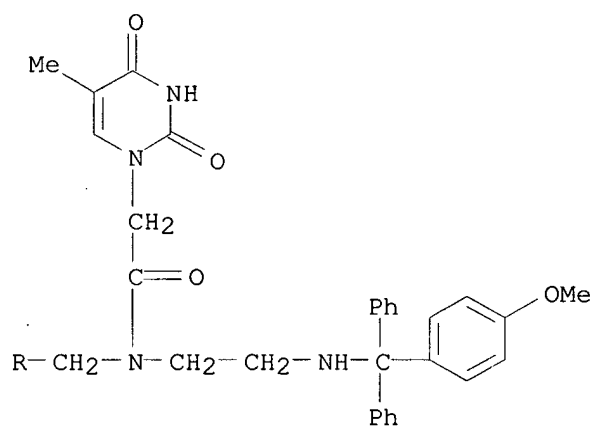
RN 227798-10-9. HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6-[(4-methoxy-1-oxido-2-pyridinyl)methoxy]-12-(4-methoxyphenyl)-6-oxido-12,12-diphenyl-2,5,8,11-tetraaza-6-phosphadodec-1-yl]-, mono[(4-methoxy-1-oxido-2-pyridinyl)methyl] ester (9CI) (CA INDEX NAME)

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=> d ibib abs hitstr 5

L13 ANSWER 5 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:235768 HCAPLUS

DOCUMENT NUMBER: 131:19274

TITLE: 2',5'-oligoadenylate-peptide nucleic acids (2-5A-PNAs) activate RNase L

AUTHOR(S): Verheijen, Jeroen C.; Van der Marel, Gijsbert A.; Van Boom, Jacques H.; Bayly, Suzanne F.; Player, Mark R.; Torrence, Paul F.

CORPORATE SOURCE: Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.

SOURCE: Bioorganic & Medicinal Chemistry (1999), 7(3), 449-455
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB To potentiate the 2-5A (2',5'-oligoadenylate)-antisense and peptide nucleic acid (PNA) approaches to regulation of gene expression, composite mols. were generated contg. both 2-5A and PNA moieties. 2-5A-PNA adducts were synthesized using solid-phase techniques. Highly cross-linked polystyrene beads were functionalized with glycine tethered through a p-hydroxymethyl-benzoic acid linker and the PNA domain of the chimeric oligonucleotide analog was added by sequential elongation of the amino terminus with the monomethoxytrityl protected N-(2-aminoethyl)-N-(adenin-1-ylacetyl)glycinate. Transition to the 2-5A domain was accomplished by coupling of the PNA chain to dimethoxytrityl protected N-(2-hydroxyethyl)-N-(adenin-1-ylacetyl)glycinate. Finally, (2-cyanoethyl)-N,N-diisopropyl-4-O-(4,4-dimethoxytrityl)butylphosphoramidite and the corresponding (2-cyanoethyl)-N,N-diisopropylphosphoramidite of 5-O-(4,4'-dimethoxytrityl)-3-O-(tert-butyl dimethylsilyl)-N6-benzoyl-adenosine were the synthons employed to add the 2 butanediol phosphate linkers and the four 2',5'-linked riboadenylates. The 5'-phosphate moiety was introduced with 2-[[[2-(4,4'-dimethoxytrityloxy)ethyl]sulfonyl]ethyl-(2-cyanoethyl)-N,N-diisopropylphosphoramidite. Deprotection with methanolic NH₃ and tetraethylammonium fluoride afforded the desired products, 2-5A-pnaA4, 2-5A-pnaA8 and 2-5A-pnaA12. When evaluated for their ability to cause the degrdn. of two different RNA substrates by the 2-5A-dependent RNase L, these new 2-5A-PNA conjugates were found to be potent RNase L activators. The union of 2-5A and PNA presents fresh opportunities to explore the biol. and therapeutic implications of these unique approaches to antisense.

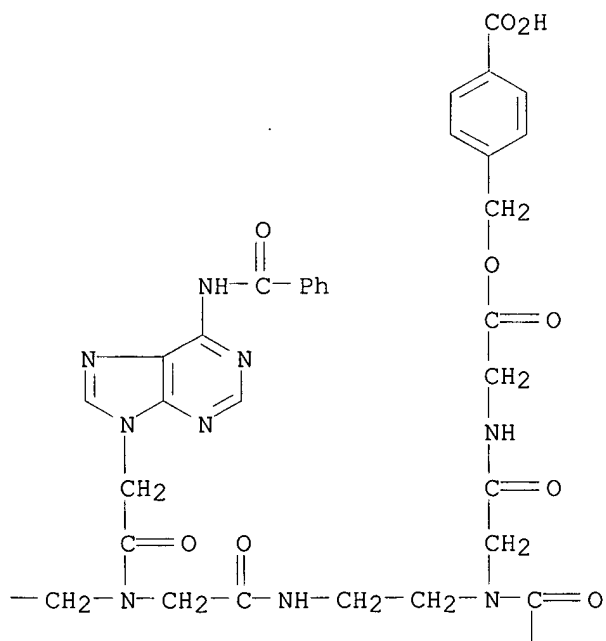
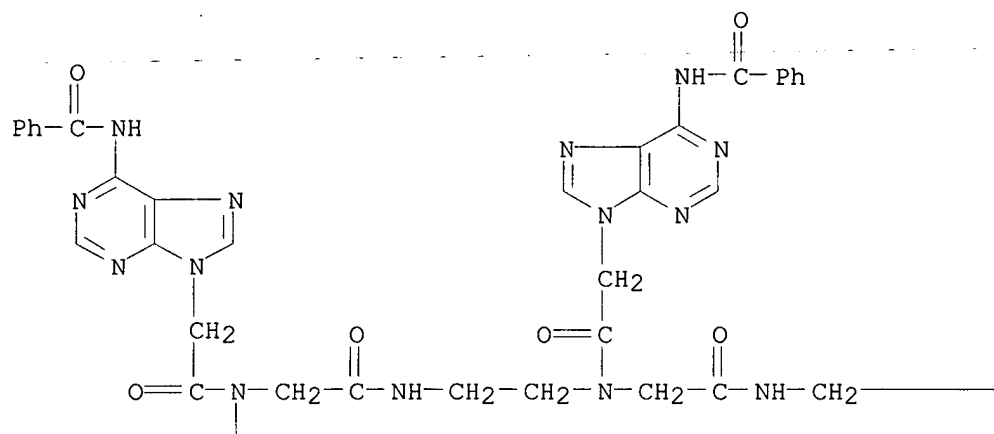
IT 225787-02-ODP, solid-supported

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

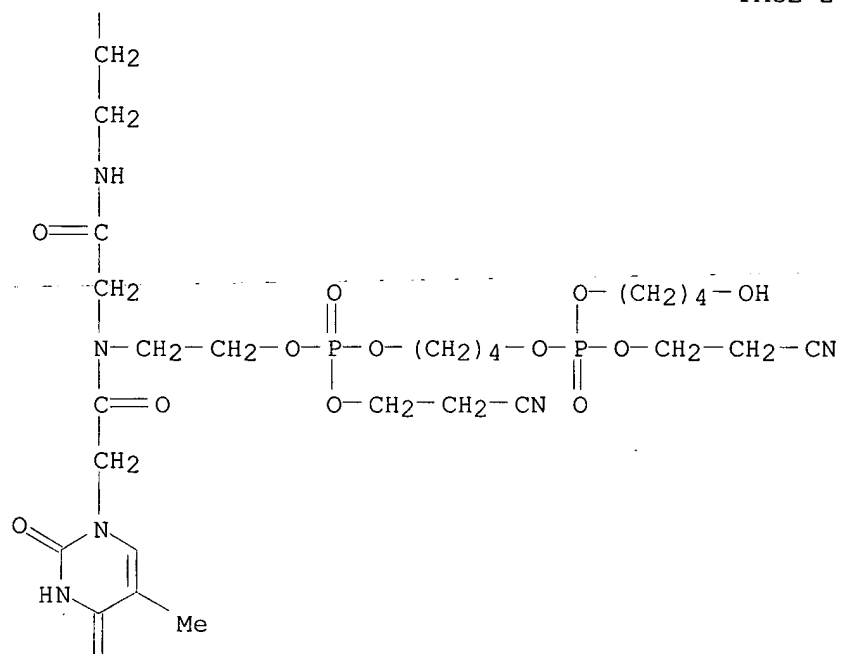
(prepn. and reaction of in the synthesis of 2',5'-oligoadenylate-peptide nucleic acids (2-5A-PNAs) for activation of RNase L)

RN 225787-02-0 HCAPLUS

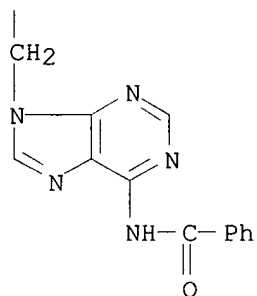
CN Peptide nucleic acid, ((deamino)(hydroxy)T-bz6A-bz6A-bz6A-bz6A)-Gly-OH, (4-carboxyphenyl)methyl ester, 5'-[2-cyanoethyl 4-[[[(2-cyanoethoxy)(4-hydroxybutoxy)phosphinyl]oxy]butyl phosphate] (9CI) (CA INDEX NAME)



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PAGE 3-A



REFERENCE COUNT:

32

THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 6

L13 ANSWER 6 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:136456 HCAPLUS

DOCUMENT NUMBER: 130:357726

TITLE: Non-radiative deactivation of the excited states of europium, terbium and ytterbium complexes by proximate energy-matched OH, NH and CH oscillators: an improved luminescence method for establishing solution hydration states

AUTHOR(S): Beeby, Andrew; Clarkson, Ian M.; Dickins, Rachel S.; Faulkner, Stephen; Parker, David; Royle, Louise; de Sousa, Alvaro S.; Williams, J. A. Gareth; Woods, Mark
CORPORATE SOURCE: Department of Chemistry, University of Durham, Durham, DH1 3LE, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1999), (3), 493-504
CODEN: JCPKBH; ISSN: 0300-9580

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The radiative rate consts. for depopulation of the excited states of closely-related series of anionic, neutral and cationic Eu, Tb and Yb complexes were measured in H2O and D2O. With the aid of selective ligand deuteration, the relative contributions of OH, NH (both amide and amine) and CH oscillators were measured and critically assessed. Quenching of the Eu 5D0 excited state by amine NH oscillators is more than twice as efficient as OH quenching. The importance of the distance between the excited Ln ion and the XH oscillator is described with recourse to published crystallog. information. The general equation, $q = A'(\Delta k_{H2O} - k_{D2O})_{corr}$ is presented and revised values of A' for Eu (1.2 ms), Tb (5 ms) and Yb (1 μ s) given, which allow for the quenching contribution of closely diffusing OH oscillators. The relevance of such studies to the hydration state of certain Gd complexes is described and clear evidence provided for a break in hydration at Gd.

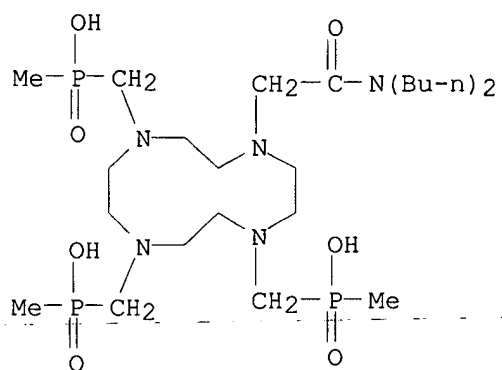
IT 145130-40-1

RL: PRP (Properties)

(complexes of Eu, Tb, Yb; non-radiative deactivation of excited states of europium, terbium and ytterbium complexes by proximate energy-matched OH, NH and CH oscillators: improved luminescence method for establishing soln. hydration states)

RN. 145130-40-1 HCAPLUS

CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris(methyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

57

THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs hitstr 7

L13 ANSWER 7 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:70167 HCAPLUS

DOCUMENT NUMBER: 128:167687

TITLE: PHONA - PNA co-oligomers: nucleic acid mimetics with interesting properties

AUTHOR(S): Peyman, Anusch; Uhlmann, Eugen; Wagner, Konrad; Augustin, Sascha; Weiser, Caroline; Will, David W.; Breipohl, Gerhard

CORPORATE SOURCE: Hoechst Marion Roussel Deutschland GmbH, Frankfurt, D-65926, Germany

SOURCE: Angewandte Chemie, International Edition in English (1998), Volume Date 1997, 36(24), 2809-2812

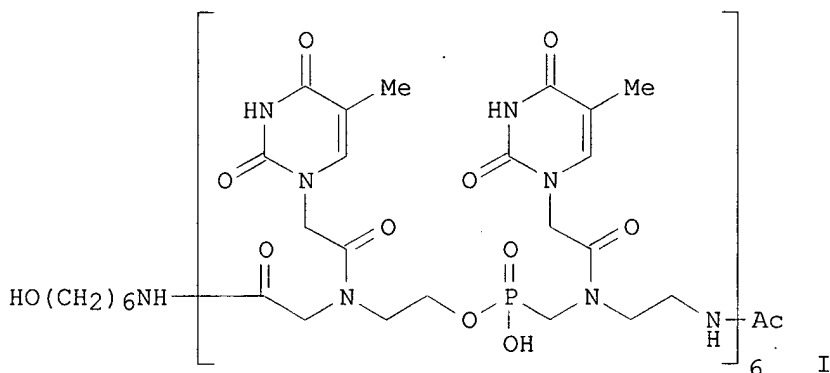
CODEN: ACIEAY; ISSN: 0570-0833

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Alternating title co-oligomer I contg. peptide nucleic acid (PNA) and (aminomethyl)phosphonic acid backbones was prepd. and melting temps. (T_m) of complexes with completely or partially complementary DNA measured. The binding properties of I with complementary DNA are very similar to those of PNAs, but the co-oligomer I has a much better water soly.

IT 202914-68-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

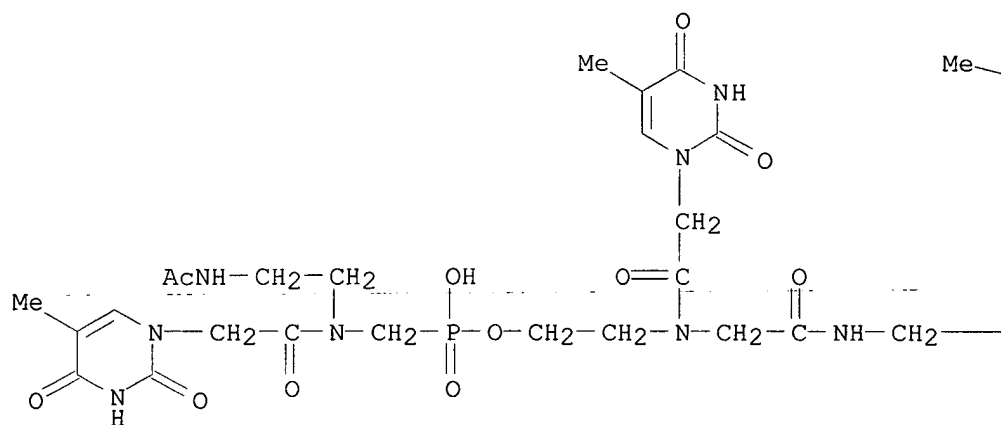
RN 202914-68-9 HCAPLUS

CN Phosphonic acid, [2,8,14,20,26,31,37-heptakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12,24,35-trihydroxy-12,24,35-trioxido-6,18,30,41-tetraoxo-11,23,34-trioxa-2,5,8,14,17,20,26,29,31,37,40-undecaaza-12,24,35-triphosphadotetracont-1-yl]-, mono[3,9,15,21,27-pentakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11,23,36-trihydroxy-11,23-dioxido-5,17,29-trioxa-12,24-dioxo-3,6,9,15,18,21,27,30-octaaza-11,23-diphosphahexatriacont-1-yl] ester (9CI) (CA INDEX NAME)

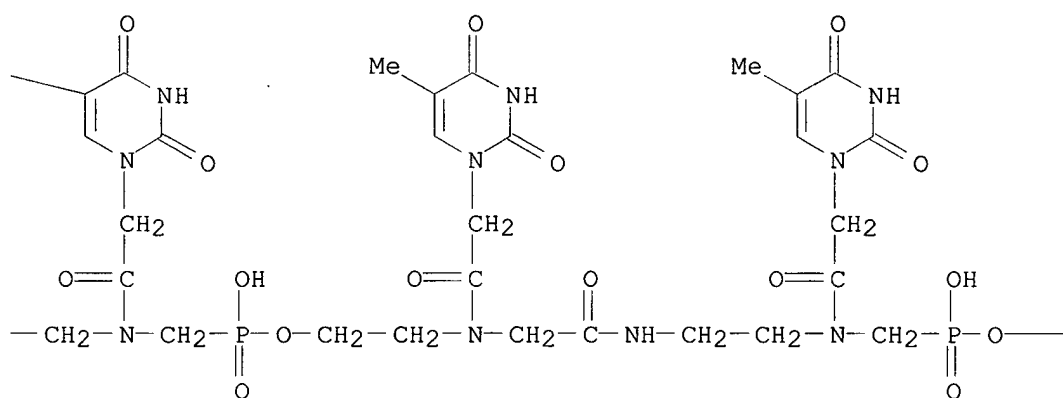
Searched by Susan Hanley 305-4053

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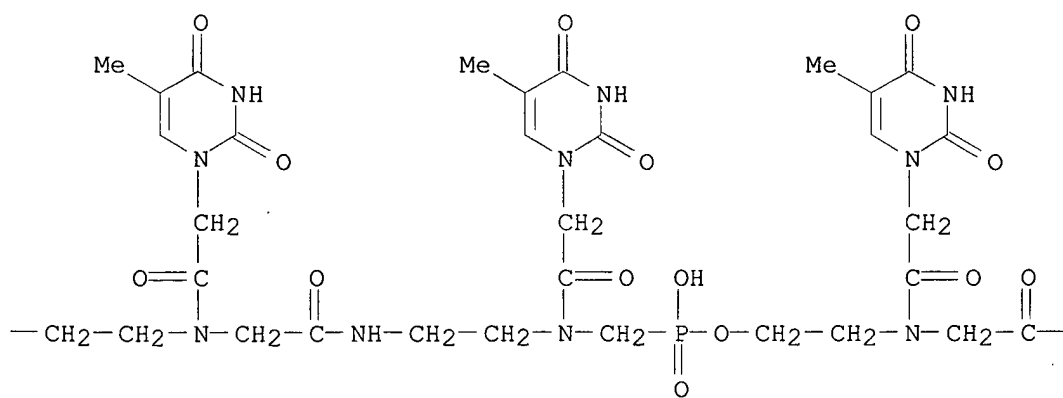
PAGE 1-A



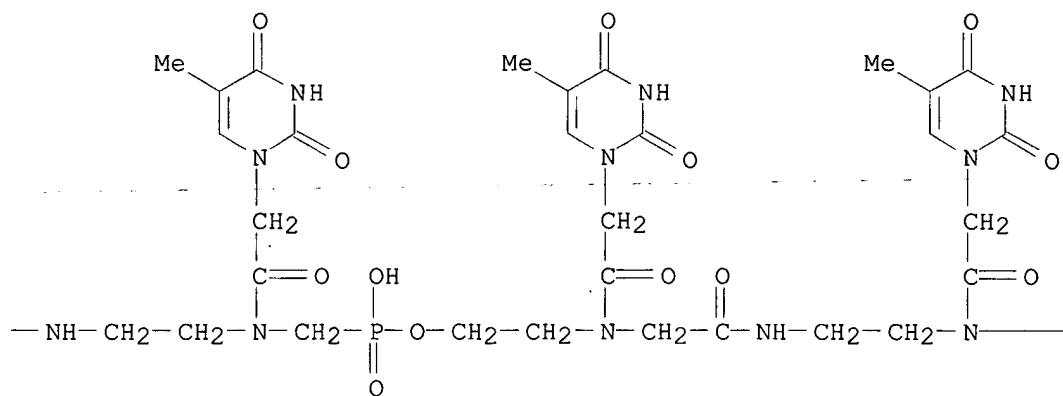
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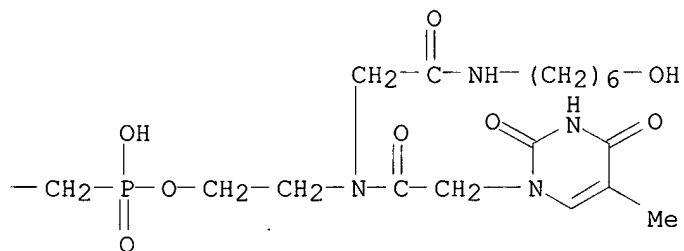
PAGE 1-C



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PAGE 1-E



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L13 ANSWER 8 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:88503 HCAPLUS

DOCUMENT NUMBER: 126:100903

TITLE: Phosphonomonoester nucleic acids, process for their preparation, and their use in molecular biology and as pharmaceuticals

INVENTOR(S): Peyman, Anuschirwan; Uhlmann, Eugen; Breipohl, Gerhard; Wallmeier, Holger

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Can. Pat. Appl., 126 pp:

CODEN: CPXXEB

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CA 2171589	AA	19960914	CA 1996-2171589	19960312
DE 19508923	A1	19960919	DE 1995-19508923	19950313
DE 19543865	A1	19970605	DE 1995-19543865	19951124
PRIORITY APPLN. INFO.:			DE 1995-19508923 A	19950313
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OTHER SOURCE(S): CASREACT 126:100903

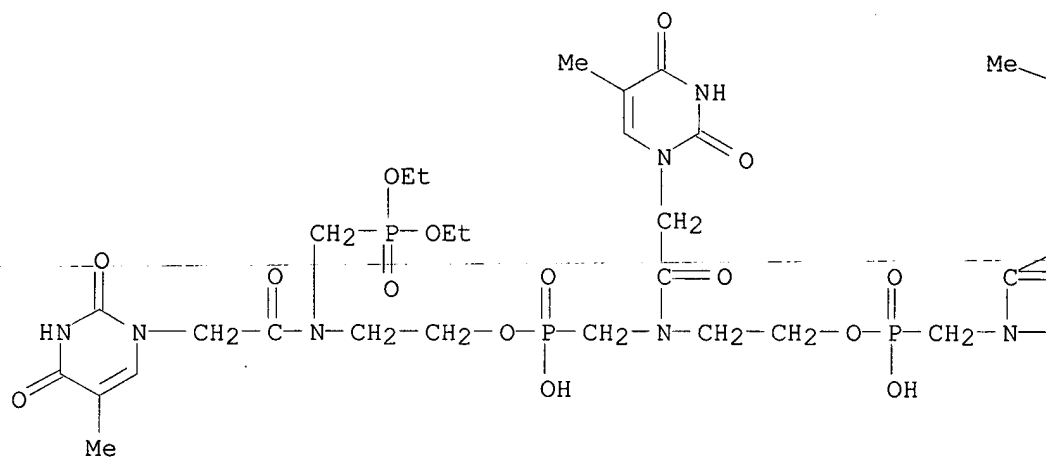
AB Novel oligonucleotide analogs which may be loosely described as phosphonomonoester analogs of peptide nucleic acids (PMENA's) and methods for their synthesis are claimed. Particularly preferred PMENA analogs are Q-[OP(:O)(OR)CH₂N(COCH₂B)CH₂CH₂]nO-Q' (n=1-25; R=OH, OEt, OPh, etc.; B=natural nucleobase; Q,Q'=H, alkyl, Ph, etc. or an oligonucleotide or modified oligonucleotide). Their application relates to use as inhibitors of gene expression (antisense oligonucleotides, ribozymes, sense oligonucleotides and triplex-forming oligonucleotides), as probes for the detection of nucleic acids and as auxiliaries in mol. biol. PMENA analog H-[OP(:O)(OH)CH₂N(COCH₂T)CH₂CH₂]9OP(:O)(OEt)OEt was prepd. and its interaction with (dA)₉ examd. by UV spectroscopy and by gel shift anal. The T_m for the PMENA analog-(dA)₉ complex was 23.degree..

IT 185670-74-0P

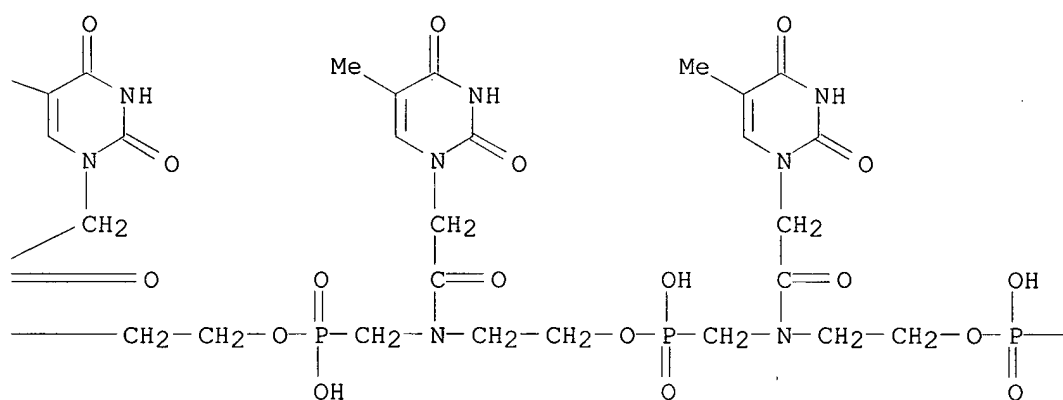
RL: PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(phosphonomonoester nucleic acids prepn. and use in mol. biol. and as pharmaceuticals)

RN 185670-74-0 HCAPLUS

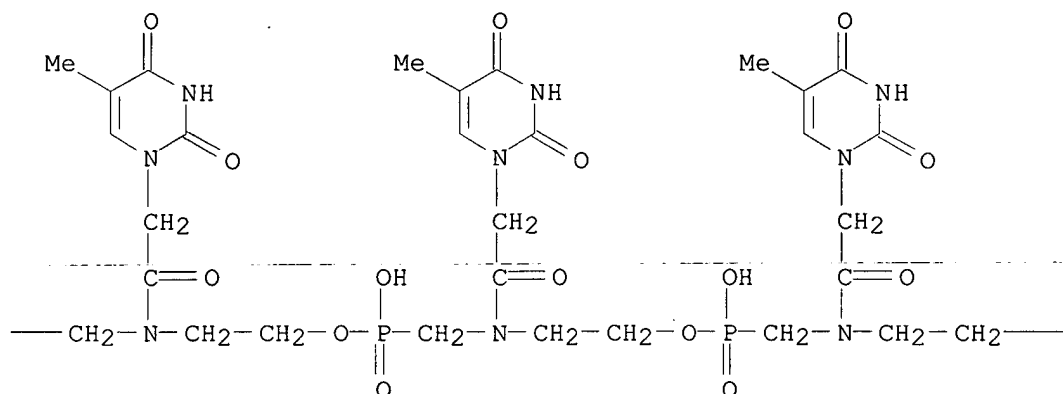
CN Phosphonic acid, [28-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6,12,18,24-tetrahydroxy-26-(2-hydroxyethyl)-6,12,18,24-tetraoxido-27-oxo-5,11,17,23-tetraoxa-2,8,14,20,26-pentaaza-6,12,18,24-tetraphosphaoctacos-1-yl]-, mono[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-23-ethoxy-5,11,17-trihydroxy-5,11,17,23-tetraoxido-6,12,18,24-tetraoxa-3,9,15,21-tetraaza-5,11,17,23-tetraphosphahexacos-1-yl] ester (9CI) (CA INDEX NAME)



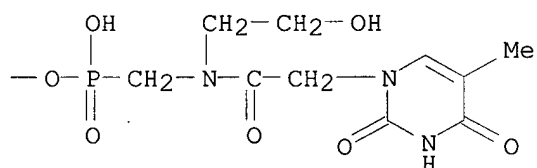
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IT 183057-63-8P 183057-66-1P 183057-94-5P
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 183058-06-2P 183058-09-5P 183058-10-8P
 183058-11-9P 183058-12-0P 183058-13-1P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

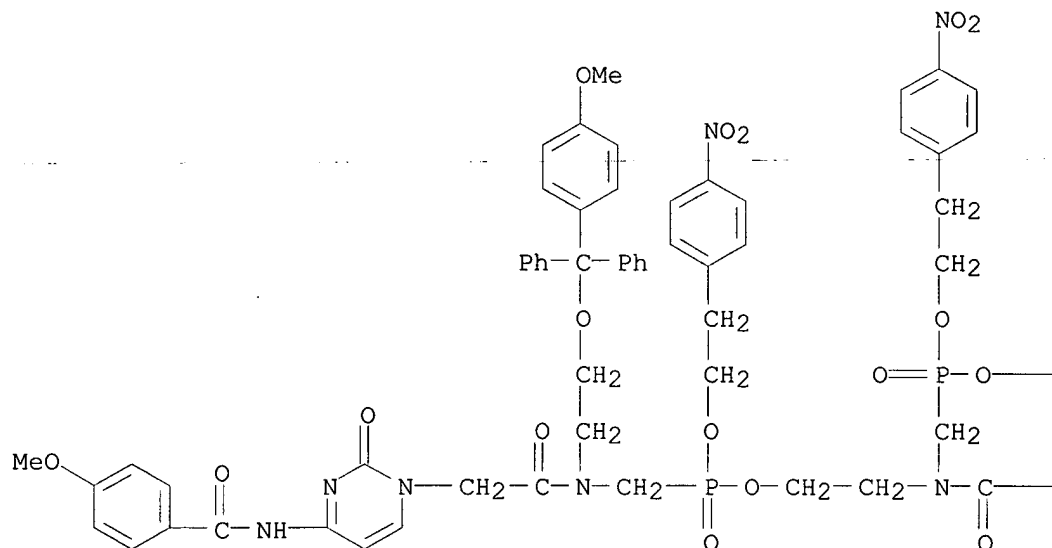
(phosphonomonoester nucleic acids prepn. and use in mol. biol. and as
 pharmaceuticals)

RN 183057-63-8 HCAPLUS

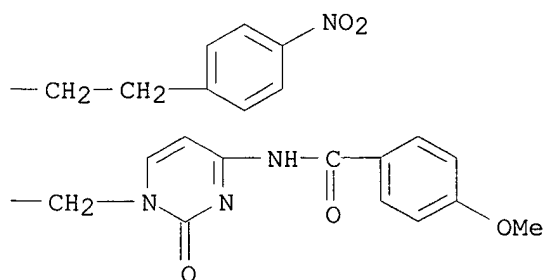
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-

pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, bis[2-(4-nitrophenyl)ethyl] ester (9CI) (CA INDEX NAME)

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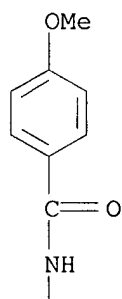
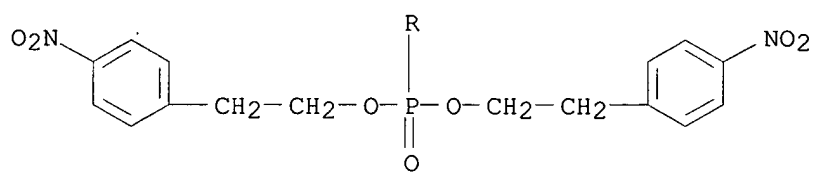
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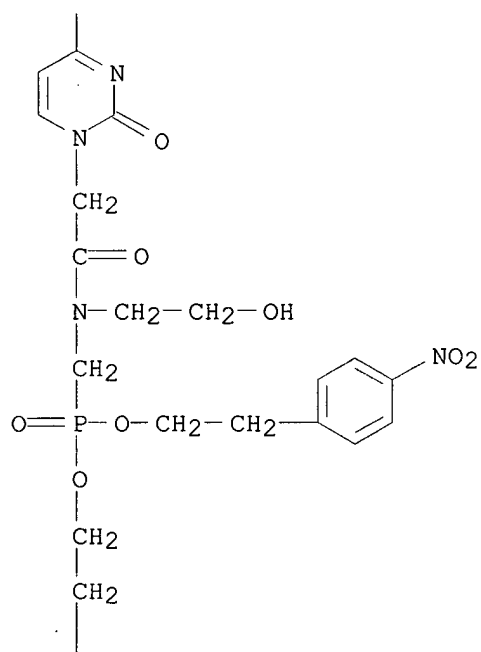
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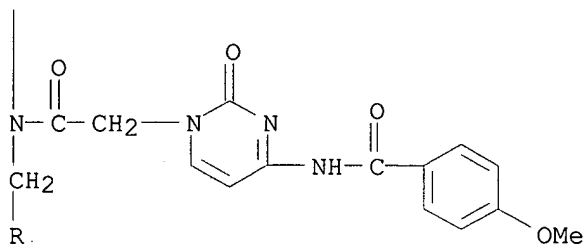
CN Phosphonic acid, [[[2-(hydroxyethyl)[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]methyl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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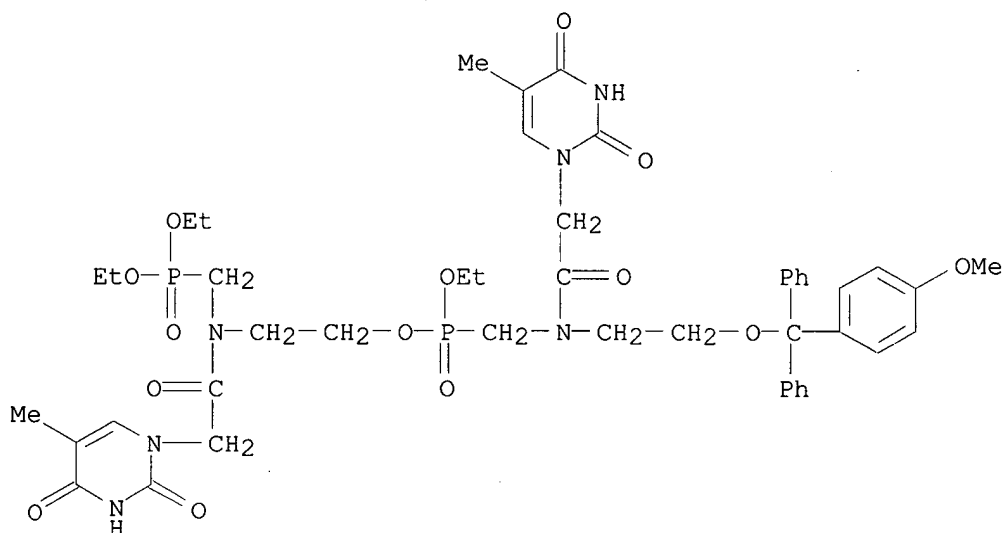
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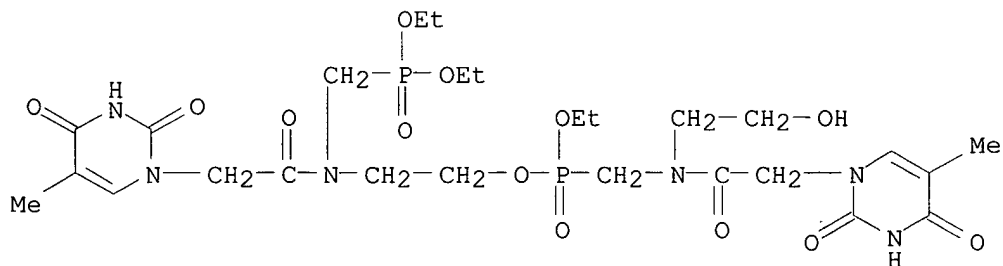
RN 183057-94-5 HCAPLUS

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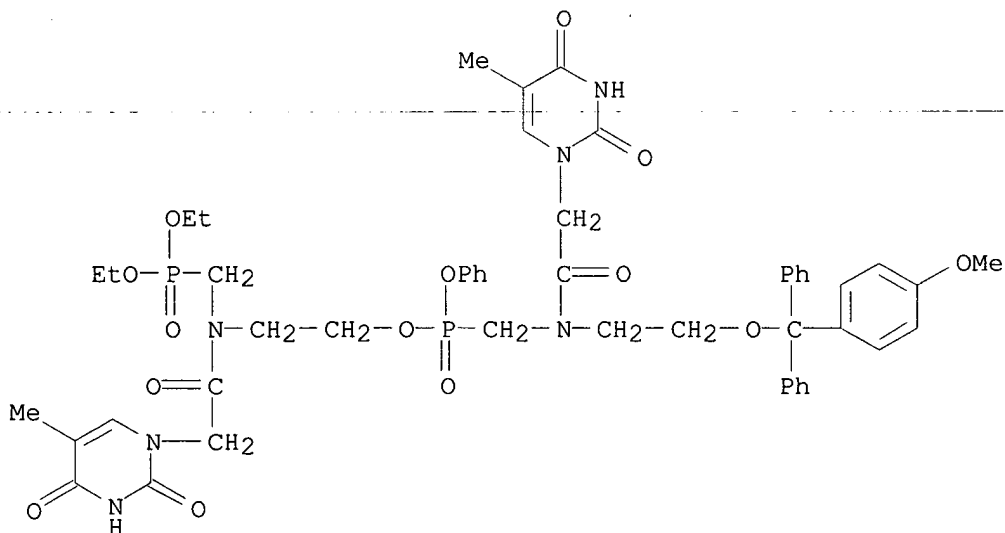
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RN 183057-99-0 HCAPLUS

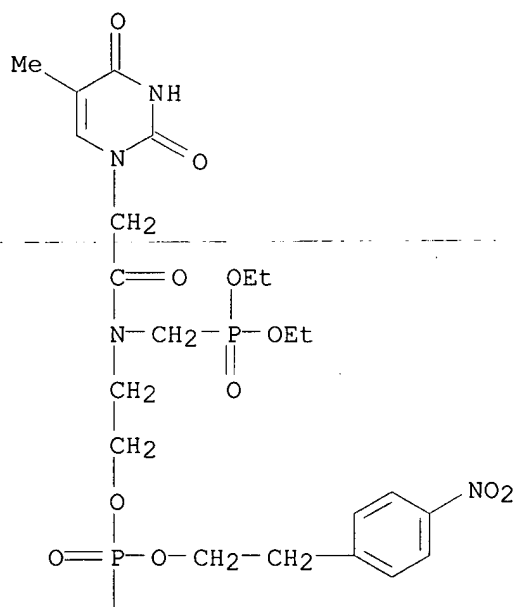
CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-oxido-6-phenoxy-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)



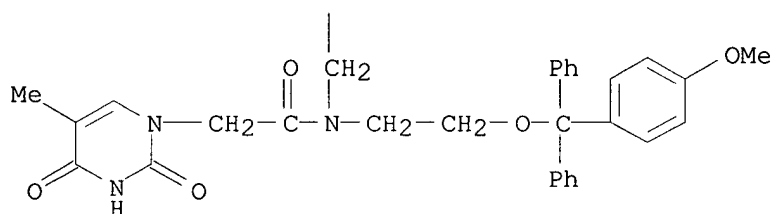
RN 183058-04-0 HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)

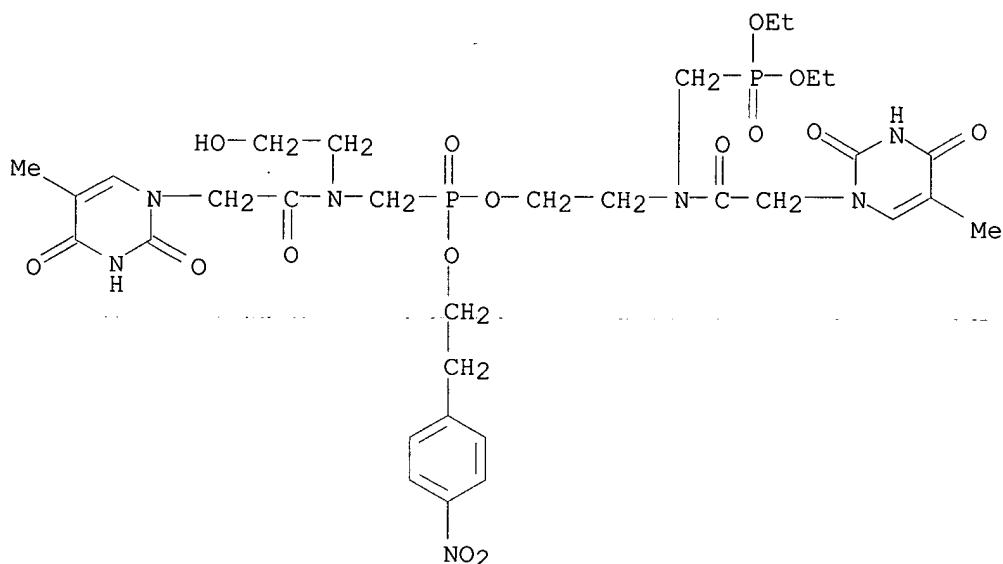
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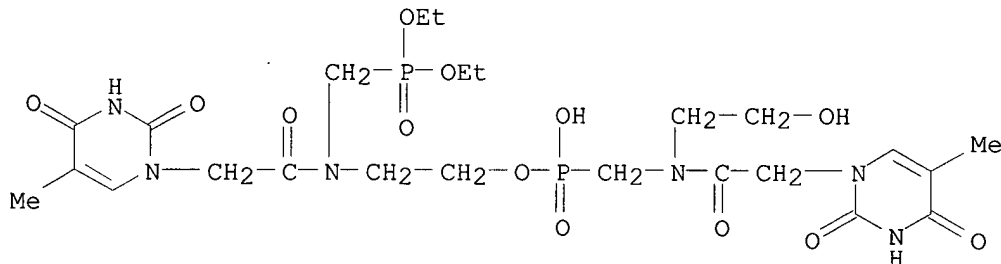


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RN 183058-09-5 HCAPLUS

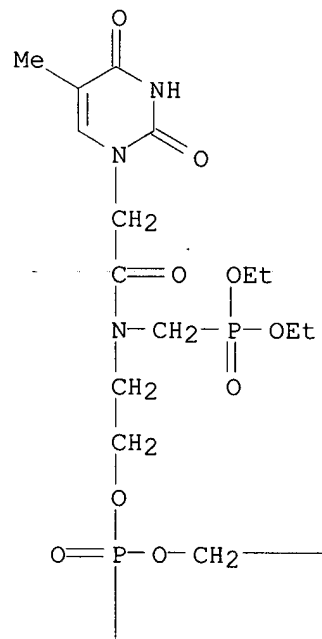
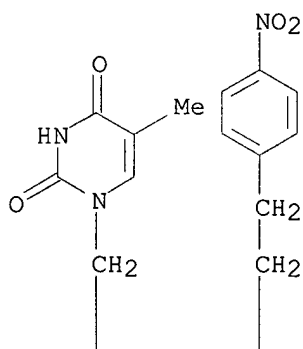
CN Phosphonic acid, [[[3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, mono[2-[[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl] ester (9CI) (CA INDEX NAME)



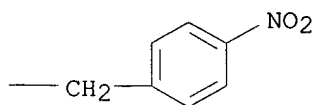
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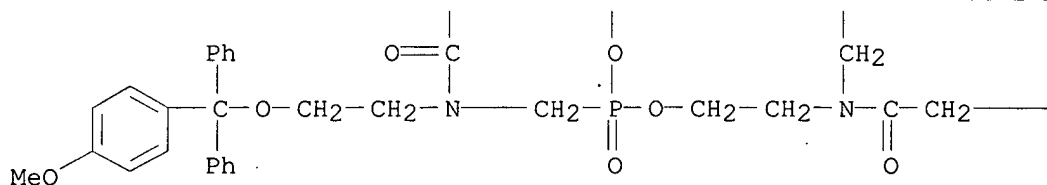
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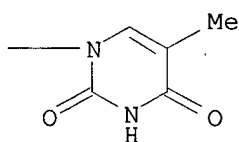
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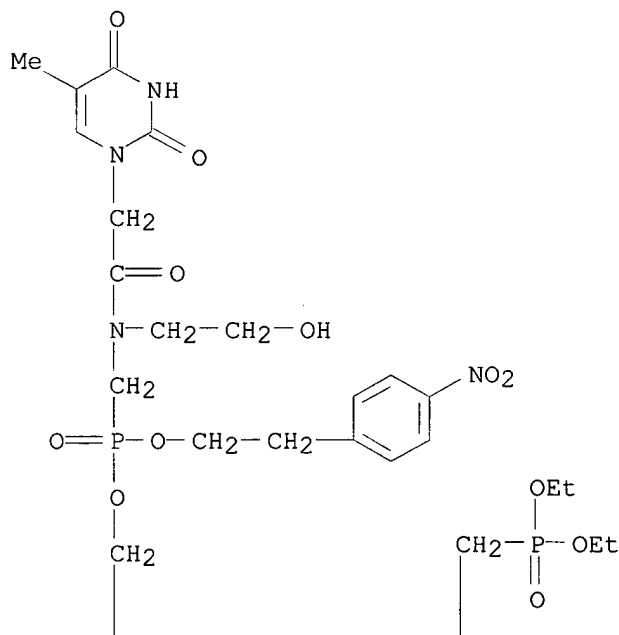
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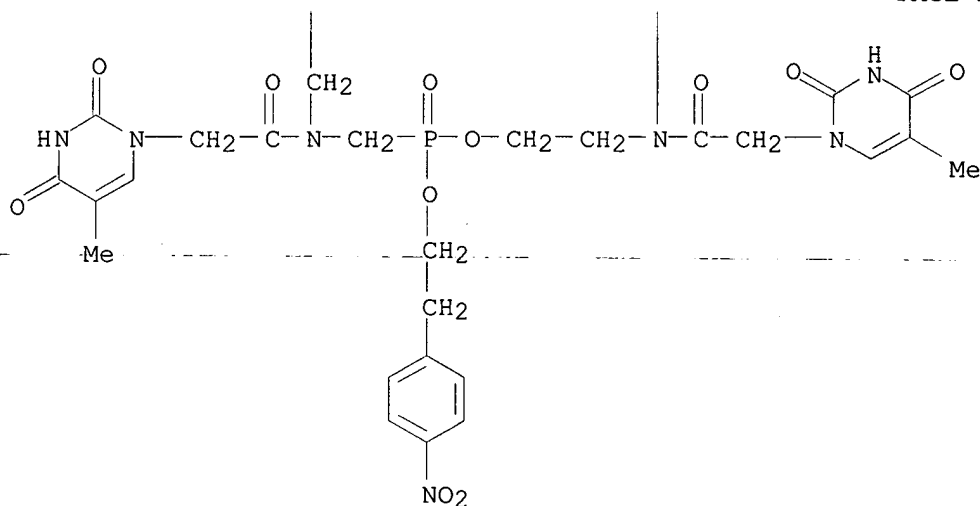
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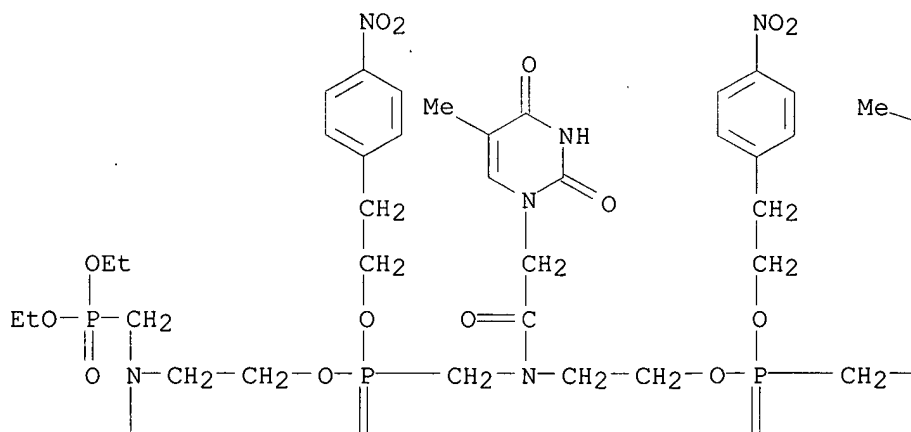
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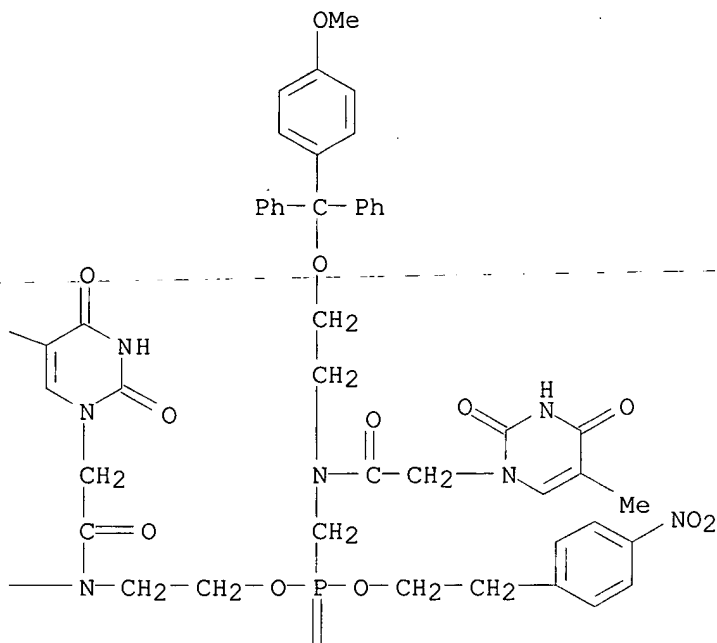
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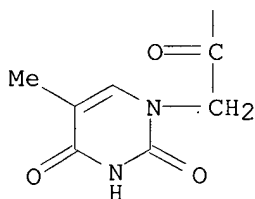
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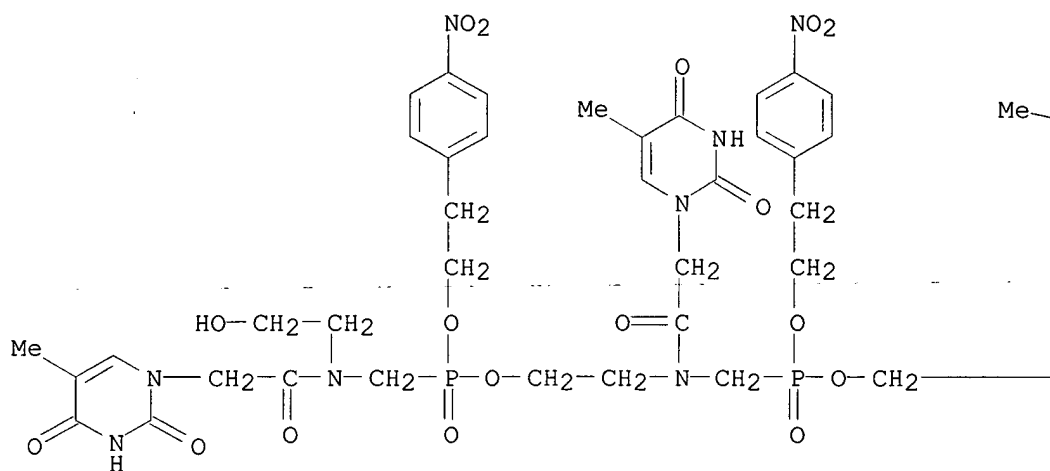
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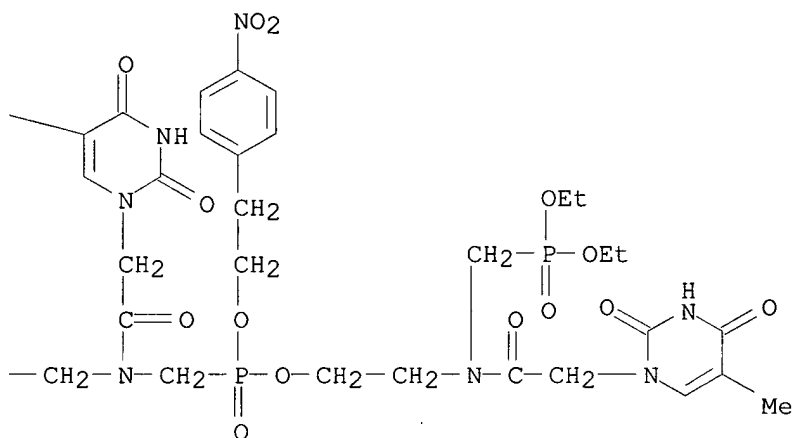
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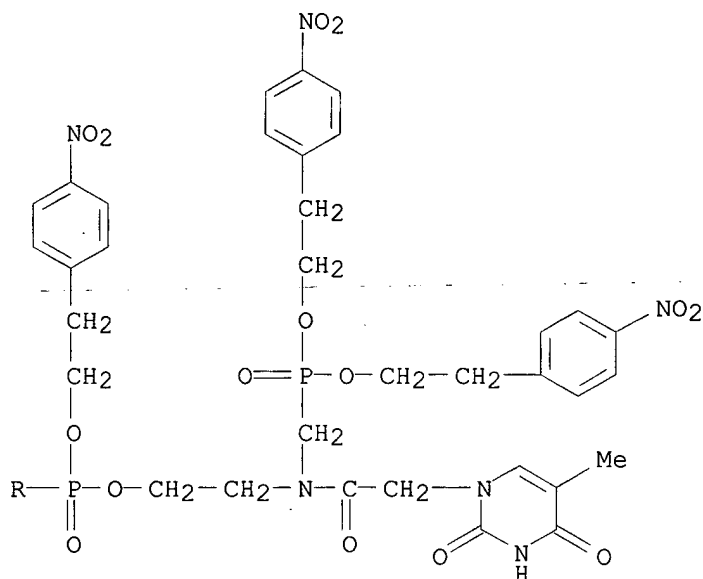
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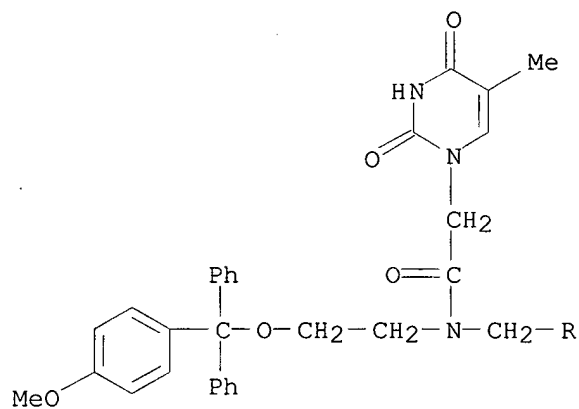
RN 183058-14-2 HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, bis[2-(4-nitrophenyl)ethyl] ester (9CI) (CA INDEX NAME)

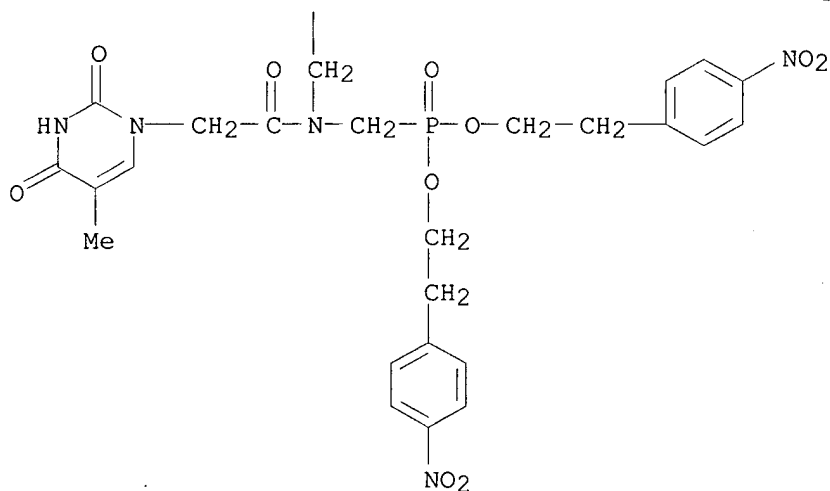
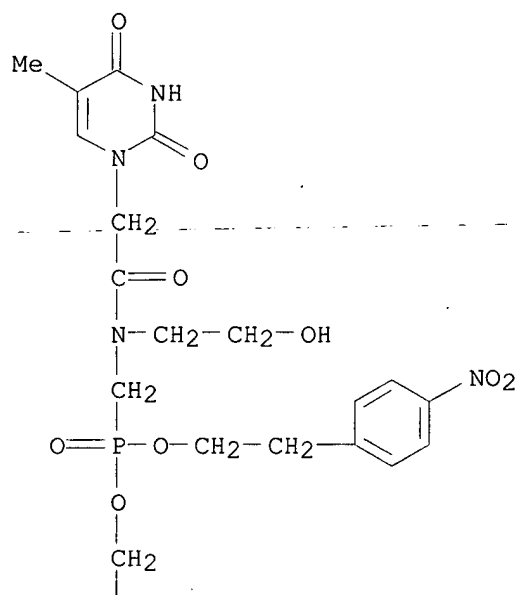
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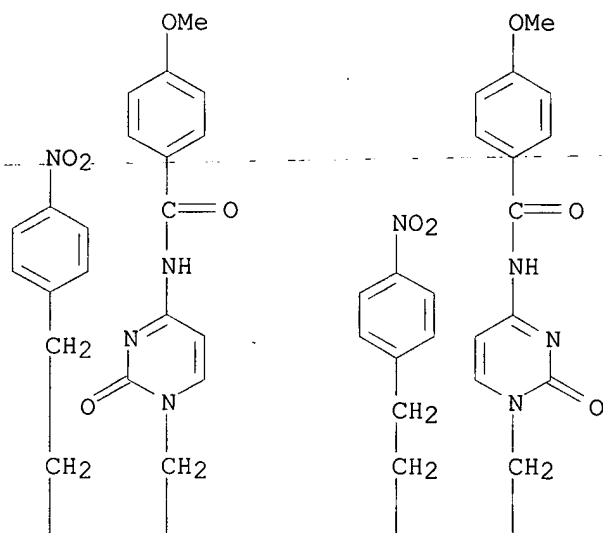


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 (CA INDEX NAME)

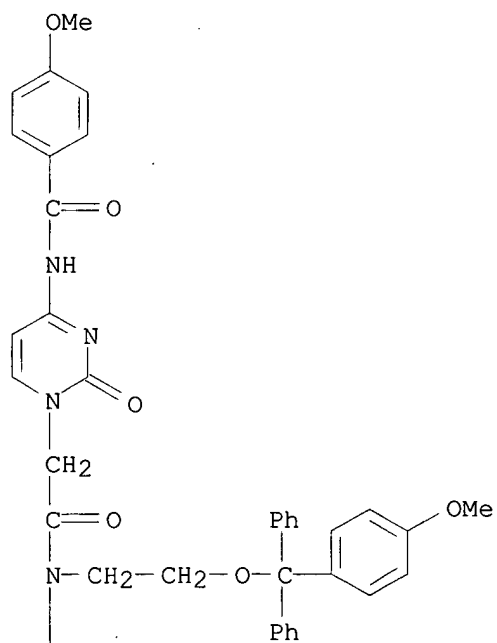


RN 183058-16-4 HCAPLUS
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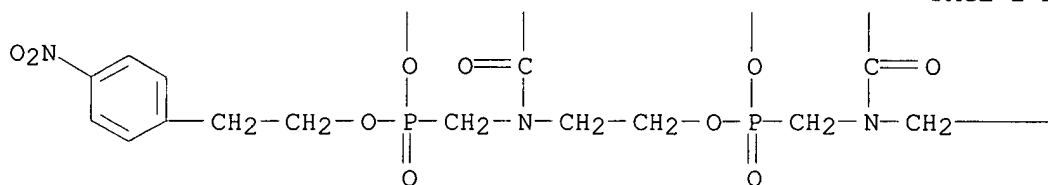
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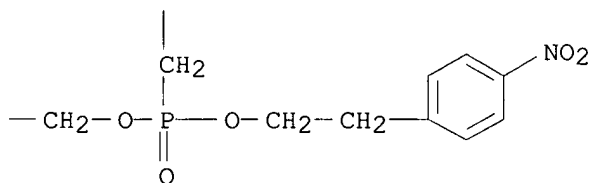
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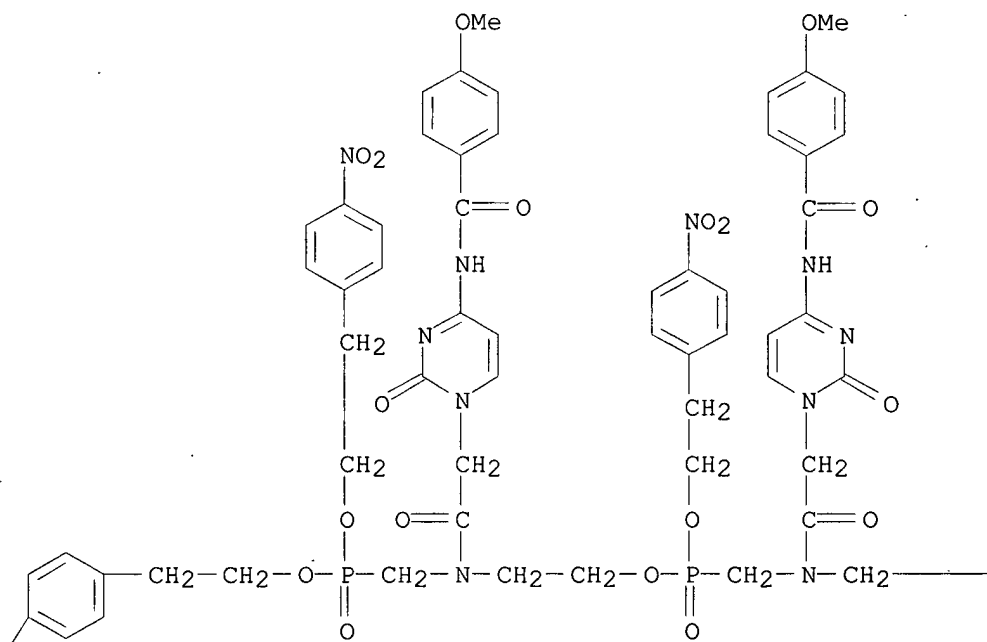


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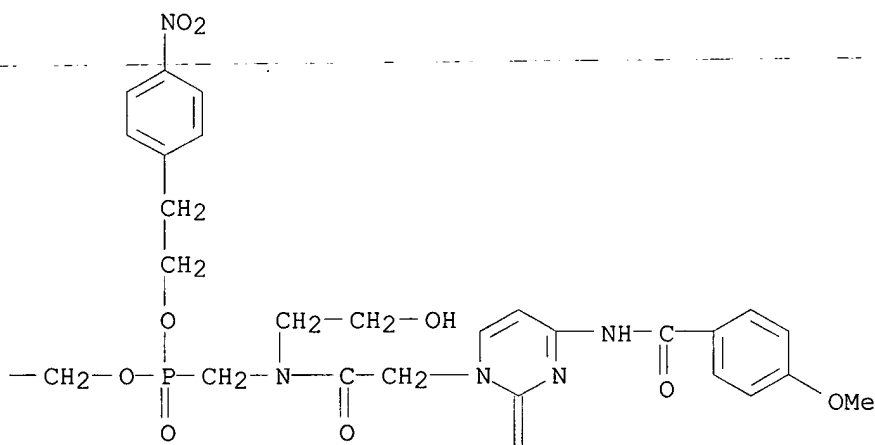


RN 183058-18-6 HCAPLUS
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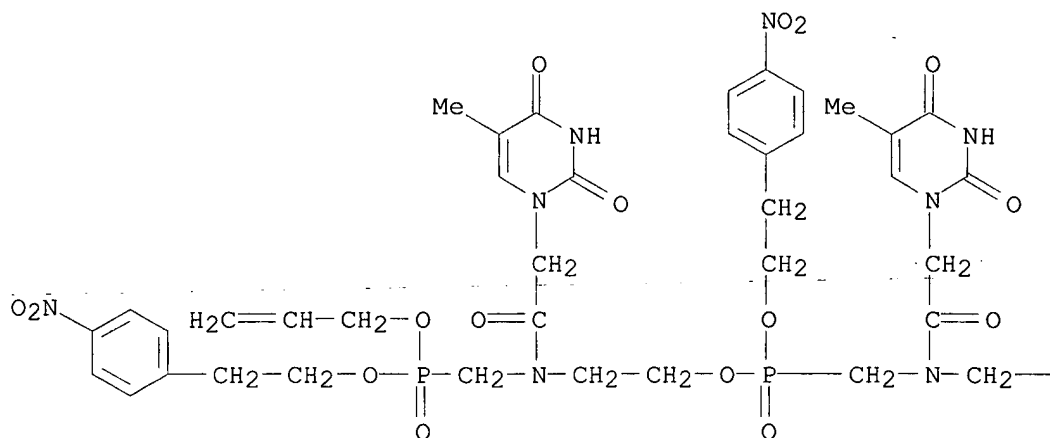


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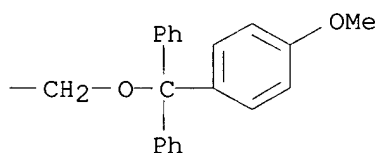


RN 185670-60-4 HCAPLUS
 CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, 2-(4-nitrophenyl)ethyl 2-propenyl ester (9CI) (CA INDEX NAME)

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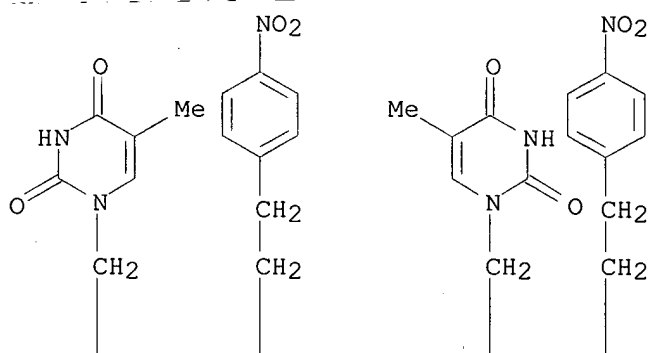
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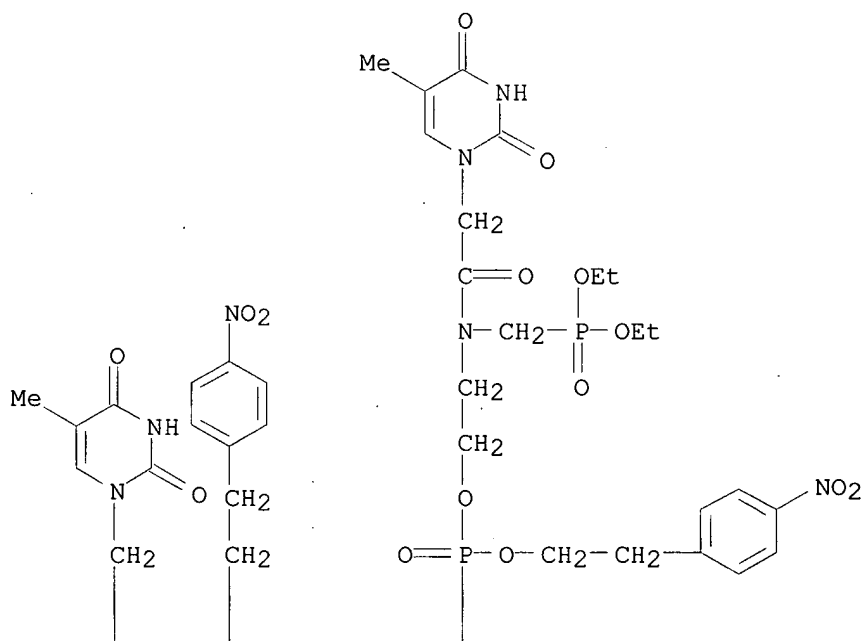
RN 185670-61-5 HCAPLUS

CN Phosphonic acid, [2,8,14-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-18-(4-methoxyphenyl)-6,12-bis[2-(4-nitrophenyl)ethoxy]-6,12-dioxido-18,18-diphenyl-5,11,17-trioxa-2,8,14-triaza-6,12-diphosphaoctadec-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

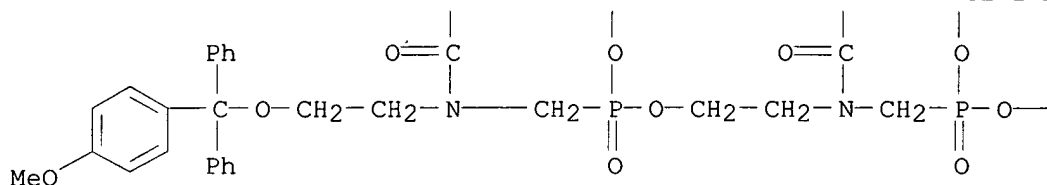
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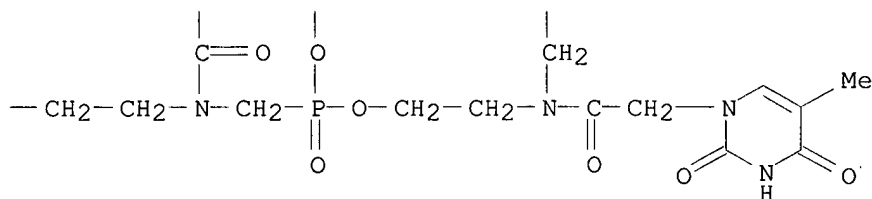
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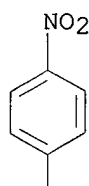
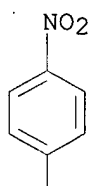
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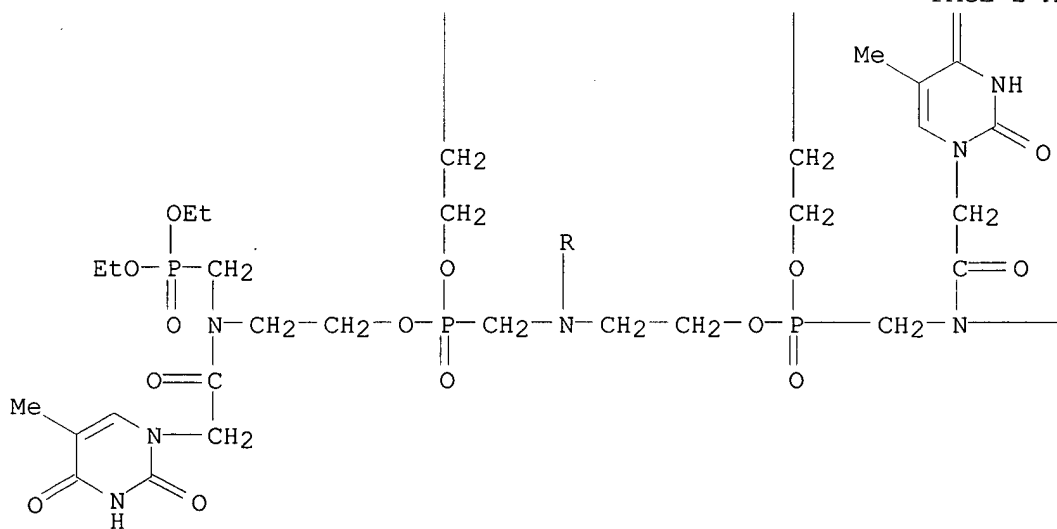
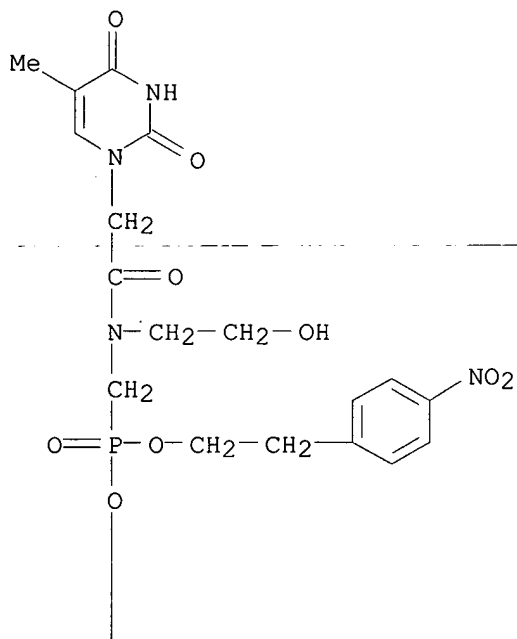


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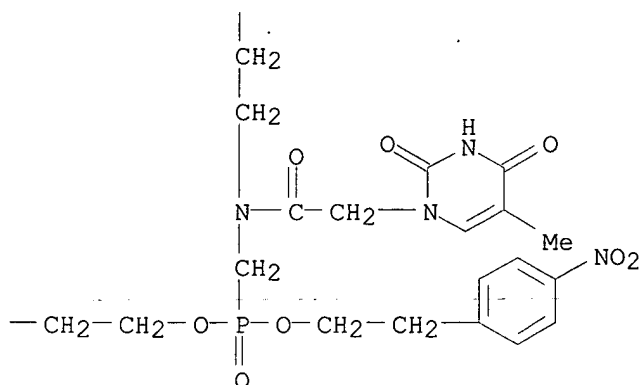
CN Phosphonic acid, [16-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14-(2-hydroxyethyl)-6,12-bis[2-(4-nitrophenyl)ethoxy]-6,12-dioxido-15-oxo-5,11-dioxo-2,8,14-triaza-6,12-diphosphahexadec-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxo-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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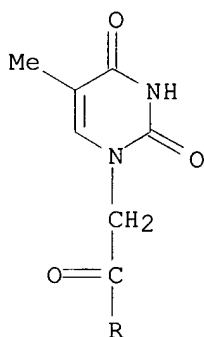




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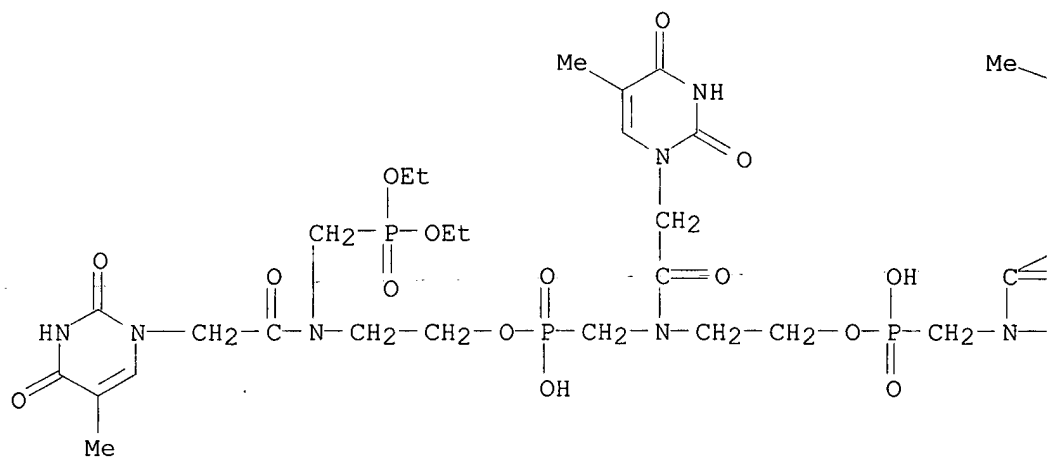


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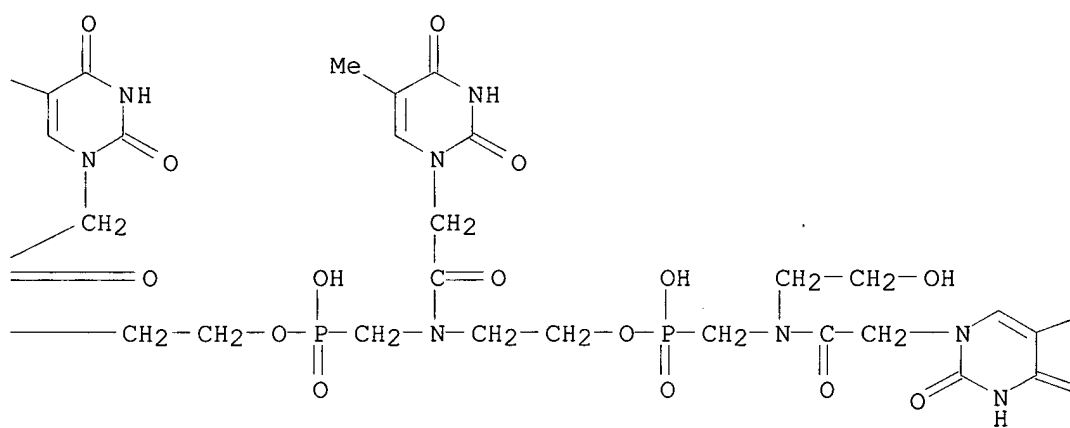


RN 185670-63-7 HCAPLUS
 CN Phosphonic acid, [16-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-
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 dihydroxy-14-(2-hydroxyethyl)-6,12-dioxido-15-oxo-5,11-dioxo-2,8,14-triaza-
 6,12-diphosphahexadec-1-yl]-, mono[3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-
 1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-hydroxy-5,11-dioxido-6,12-dioxo-3,9-
 diaza-5,11-diphosphatetradec-1-yl] ester (9CI) (CA INDEX NAME)

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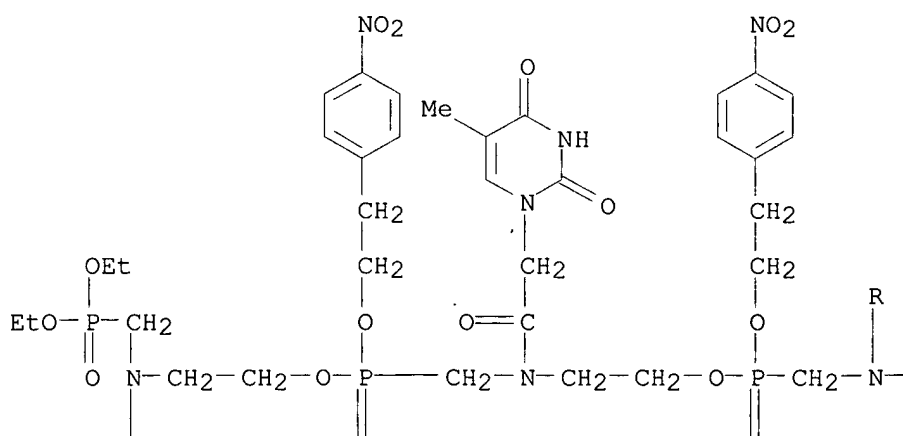
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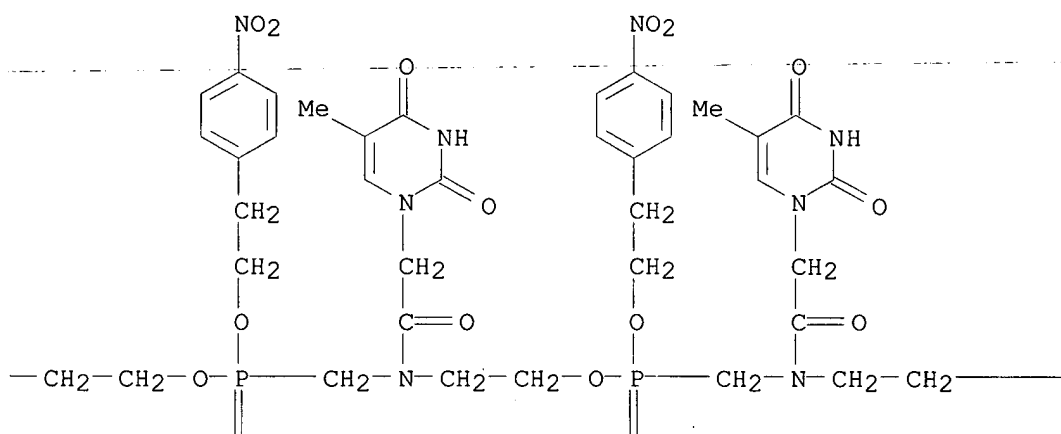
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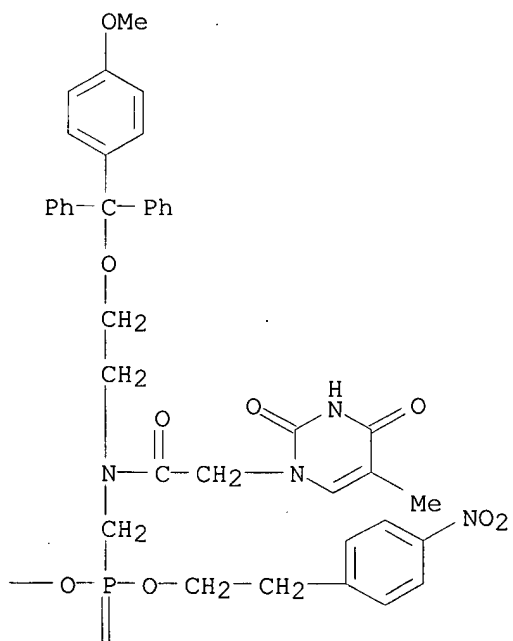
RN 185670-64-8 HCAPLUS
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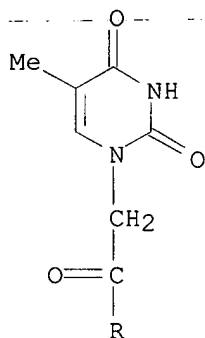
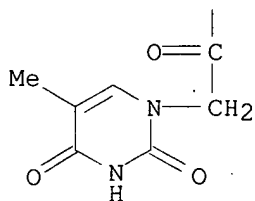
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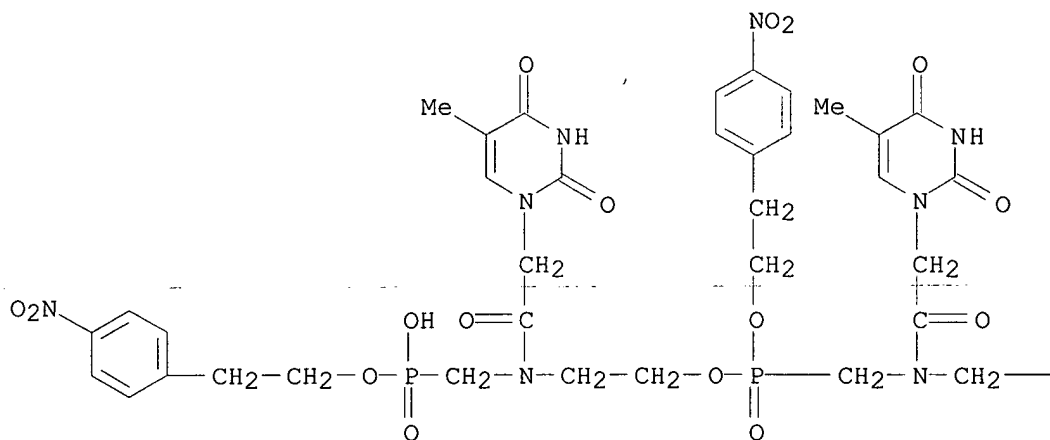


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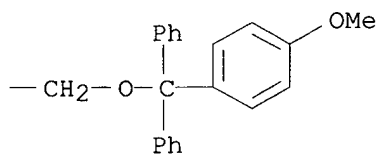


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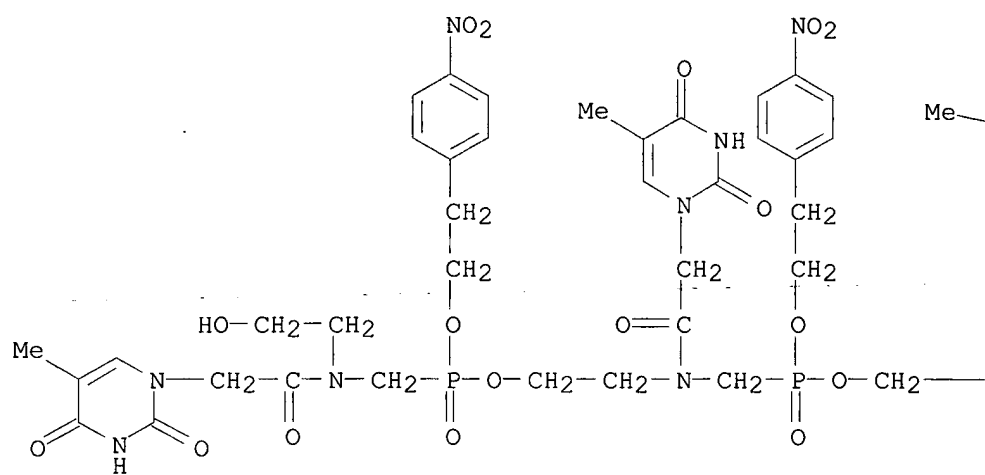
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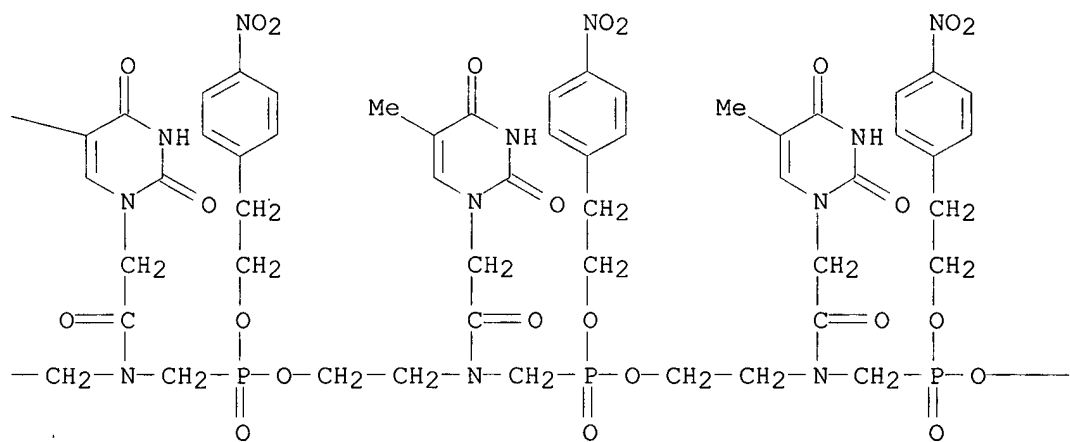
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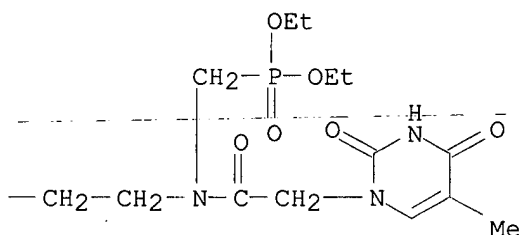
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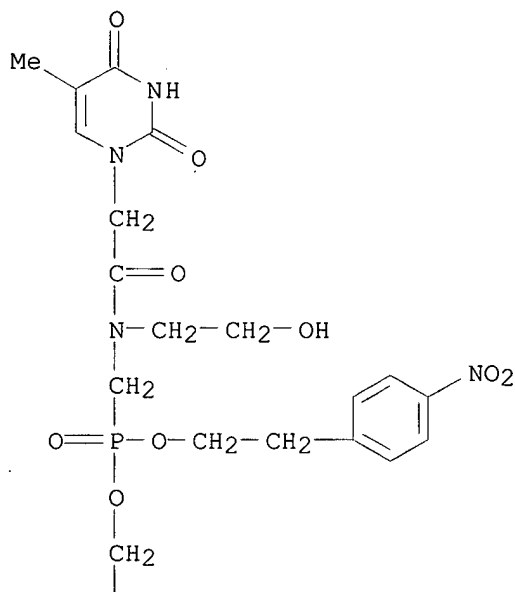


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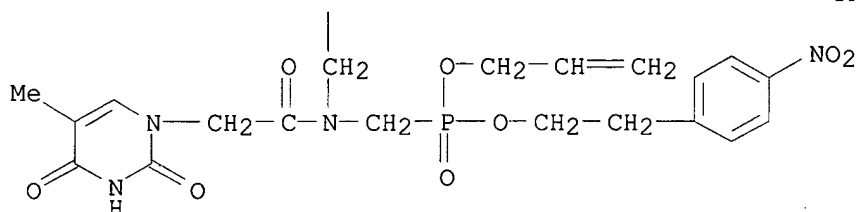


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 phosphadec-1-yl]-, 2-(4-nitrophenyl)ethyl 2-propenyl ester (9CI) (CA
 INDEX NAME)

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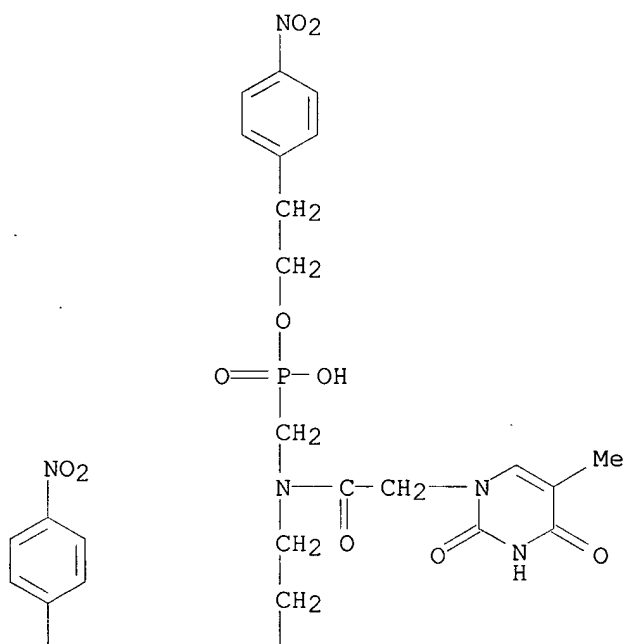
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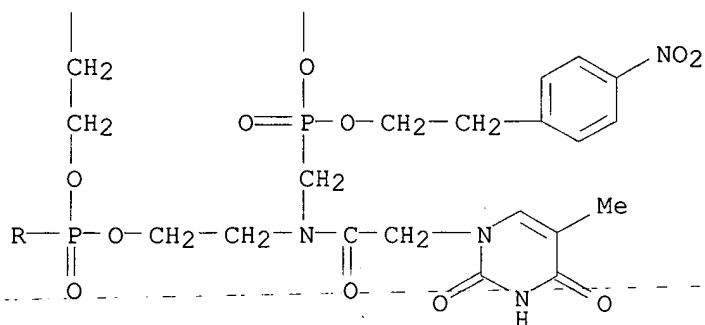
185670-68-2 HCAPLUS

Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl][[hydroxy[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

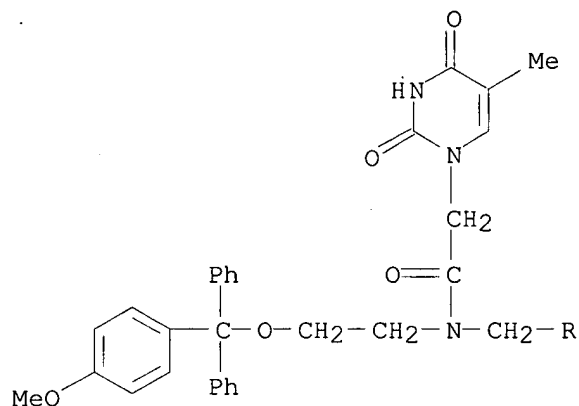
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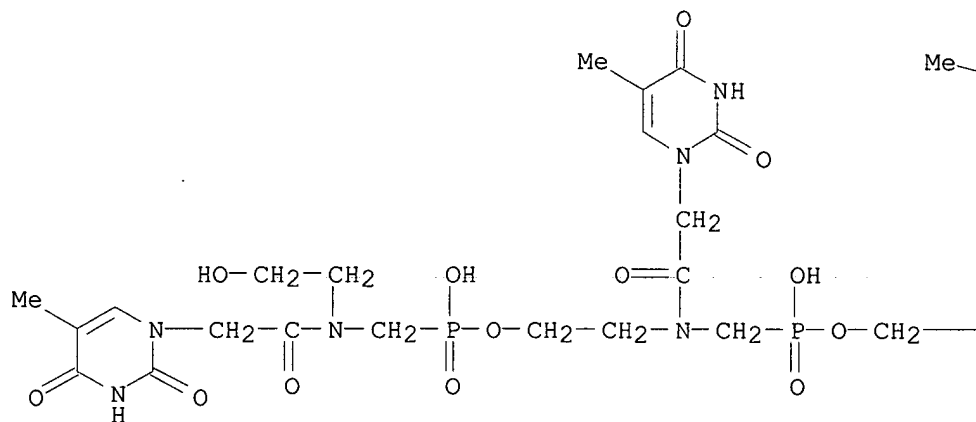
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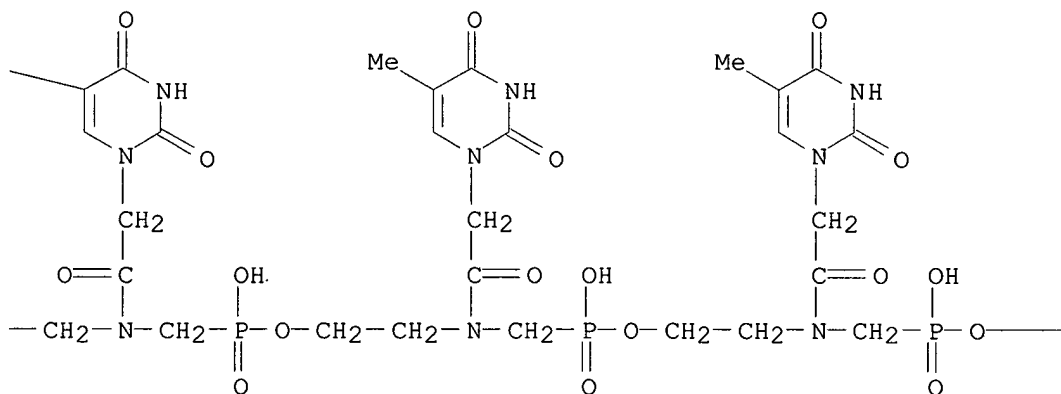
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(CA INDEX NAME)

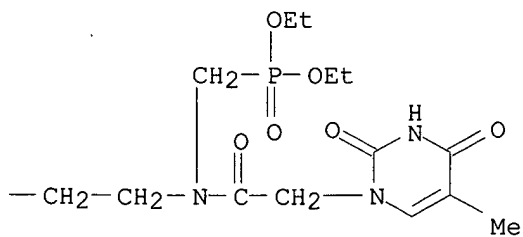
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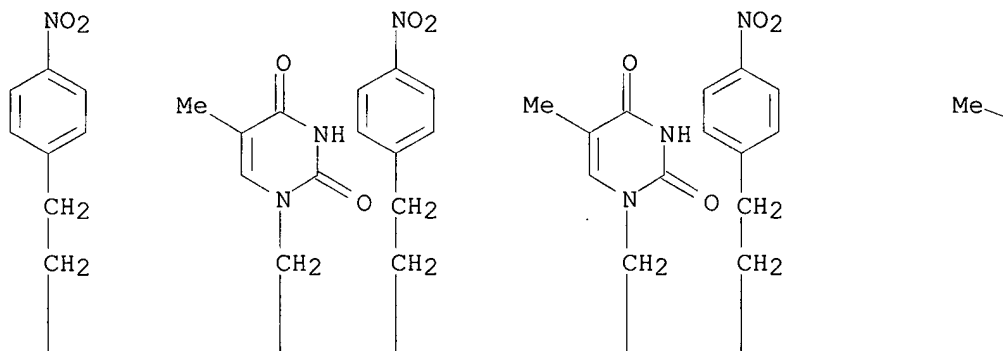
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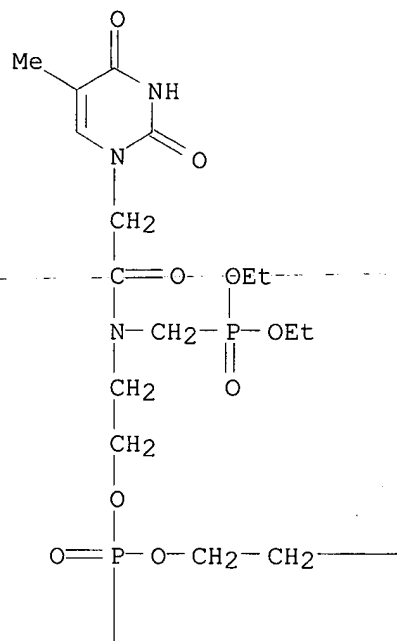
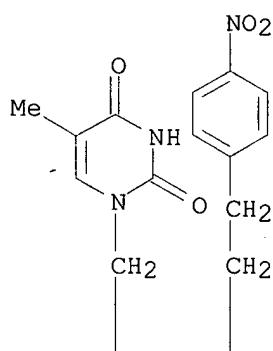
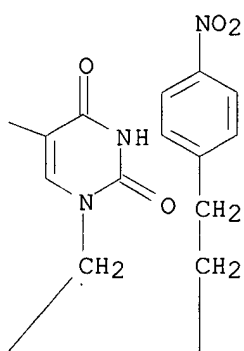
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CN Phosphonic acid, [2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetracos-1-yl]-, 2-(4-nitrophenyl)ethyl 3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-17-ethoxy-5,11-bis[2-(4-nitrophenyl)ethoxy]-5,11,17-trioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl ester (9CI) (CA INDEX NAME)

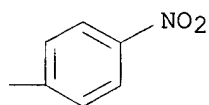
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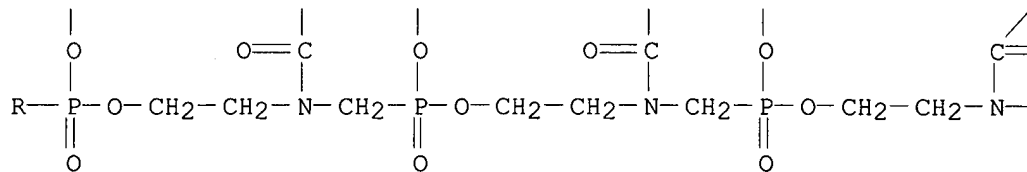
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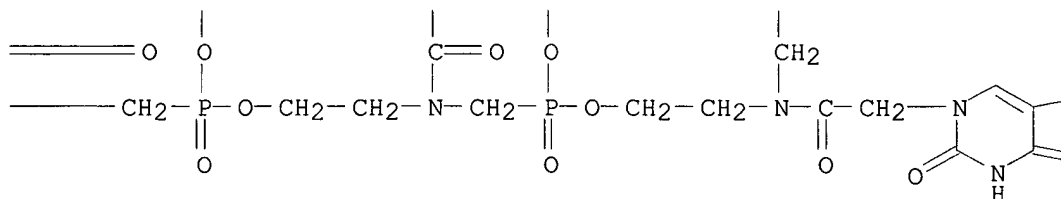
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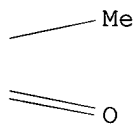
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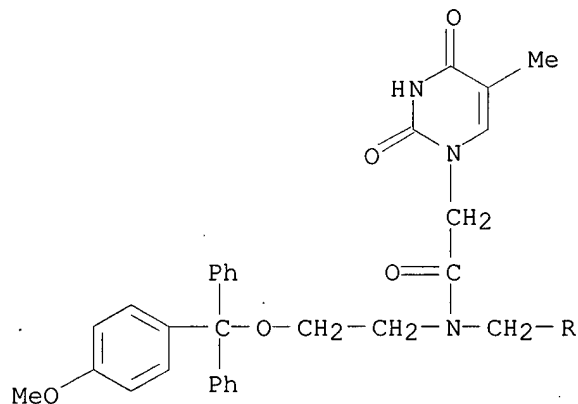
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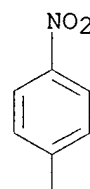
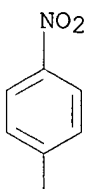
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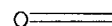
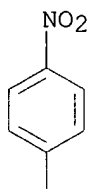
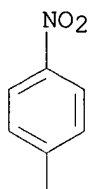
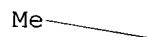
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pyrimidinyl)acetyl]-17-ethoxy-5,11-bis[2-(4-nitrophenyl)ethoxy]-5,11,17-trioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl ester (9CI) (CA INDEX NAME).

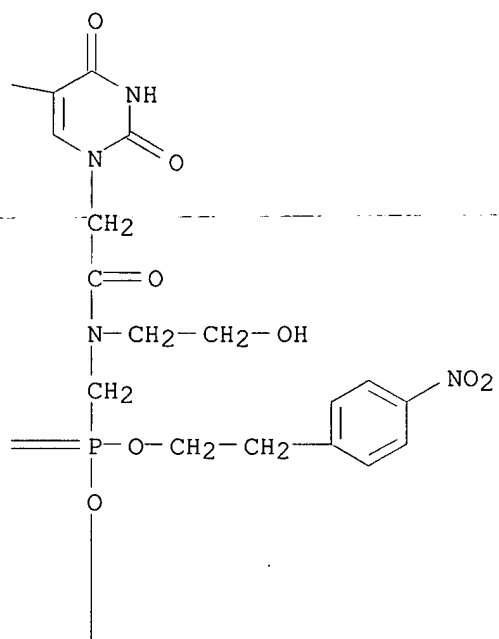
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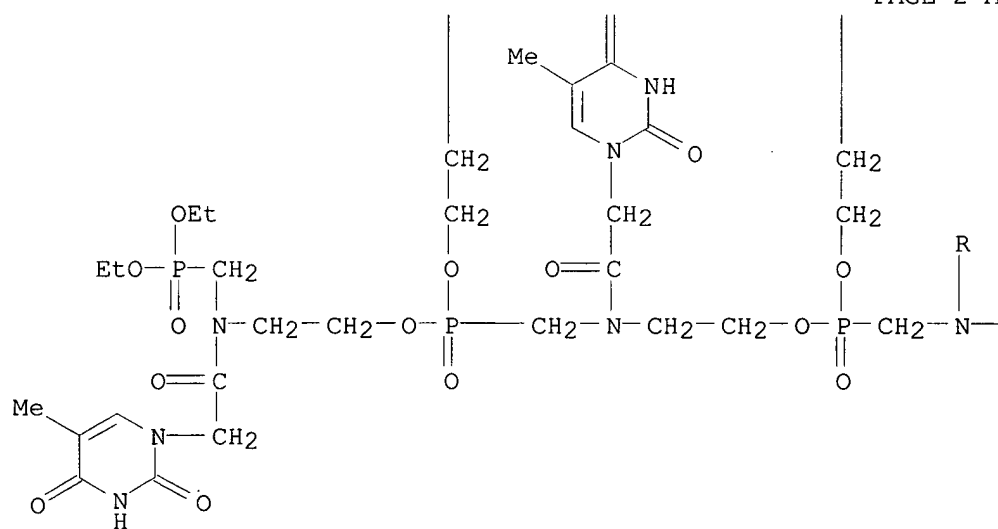
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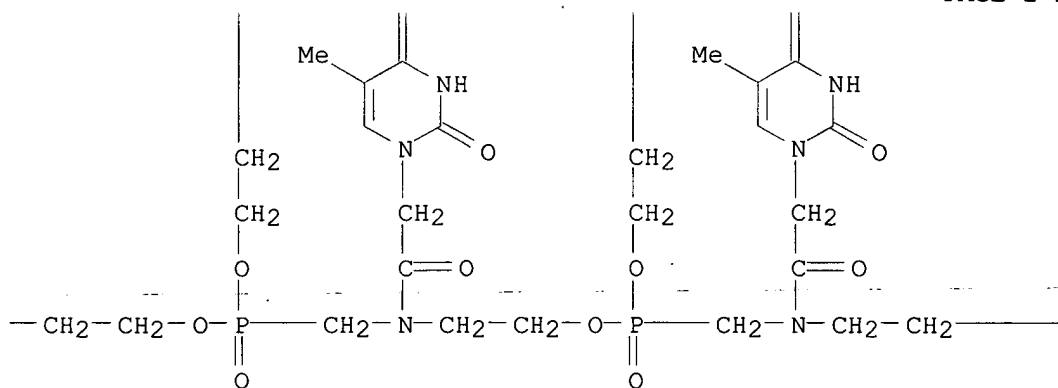
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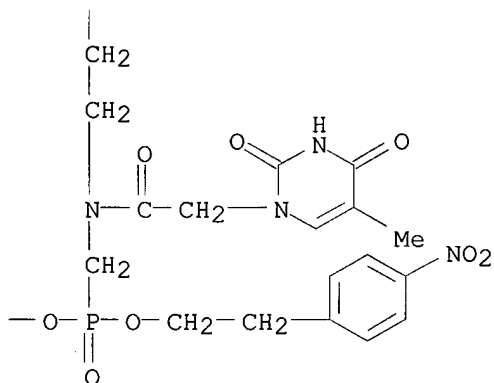
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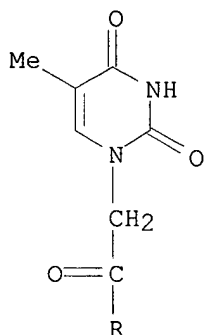
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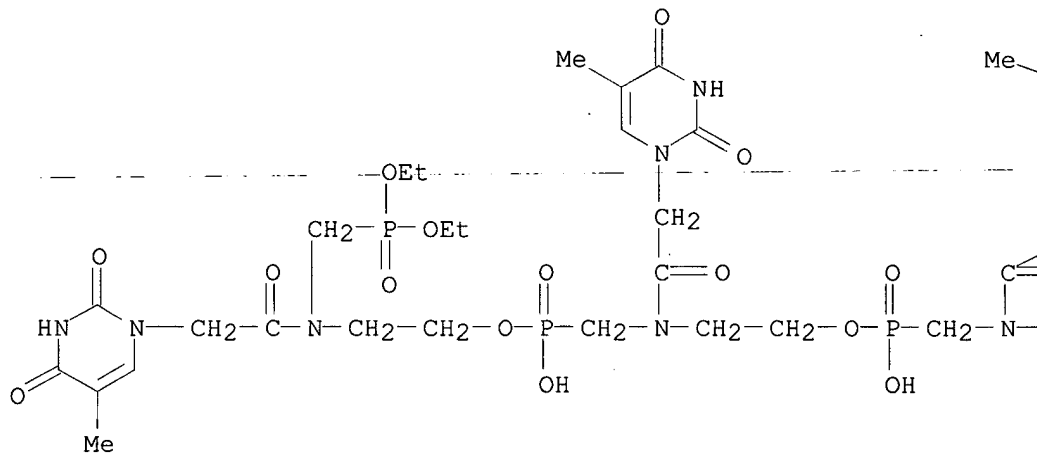
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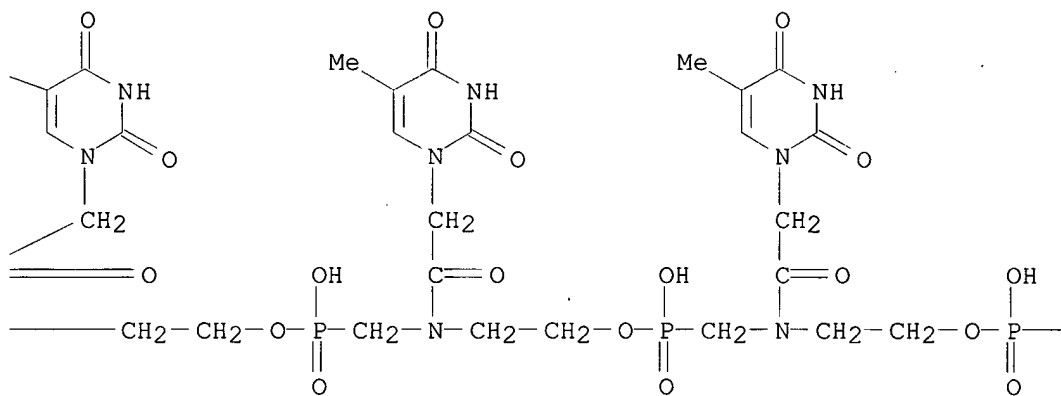
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 trioxa-2,8,14,20-tetraaza-6,12,18-triphosphadocos-1-yl]-,

mono[3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-17-ethoxy-5,11-dihydroxy-5,11,17-trioxido-6,12,18-trioxa-3,9,15-triaza-5,11,17-triphosphaeicos-1-yl] ester (9CI) (CA INDEX NAME)

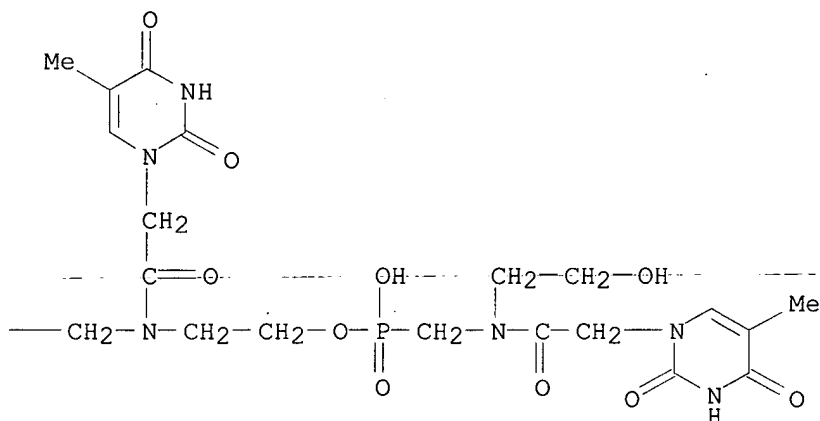
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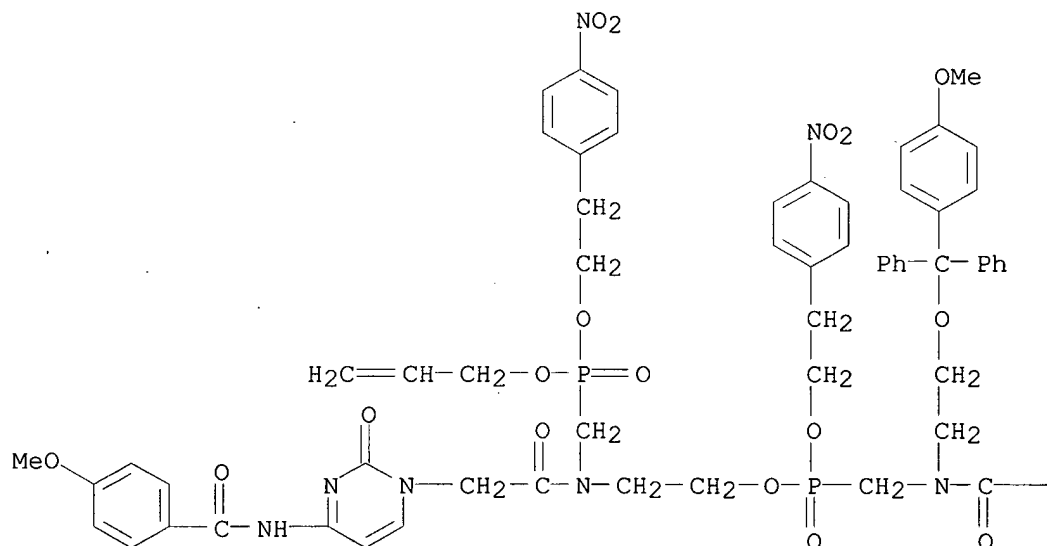
PAGE 1-C

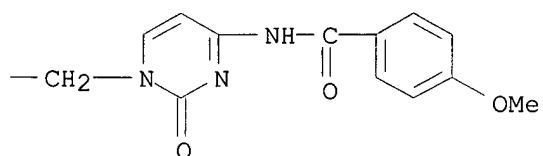


RN 185670-95-5 HCAPLUS

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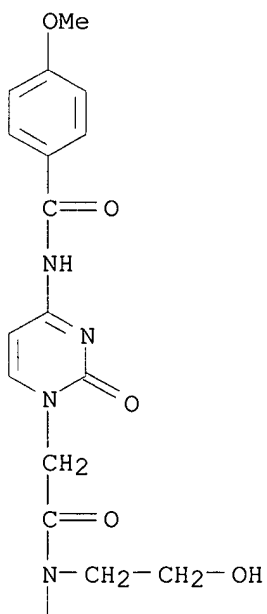
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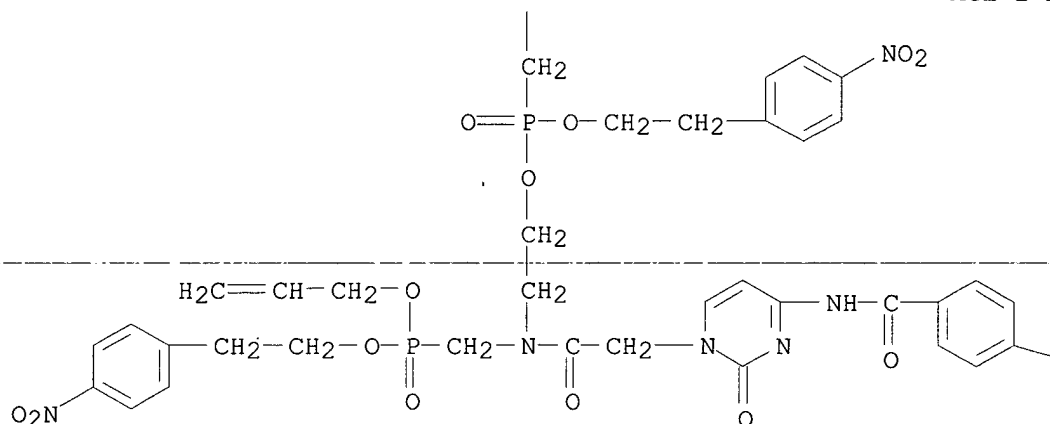




RN 185670-96-6 HCAPLUS

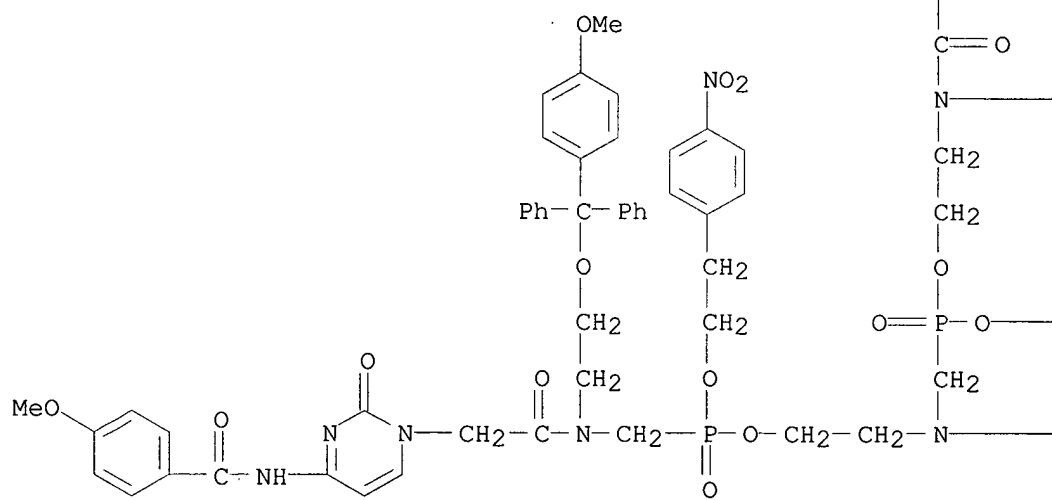
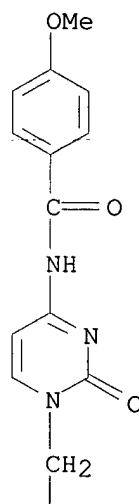
CN Phosphonic acid, [[(2-hydroxyethyl)[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]methyl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[2-(4-nitrophenyl)ethoxy](2-propenyloxy)phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

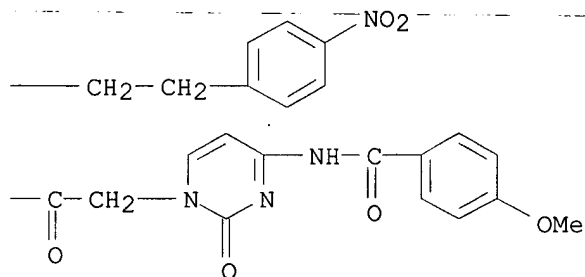
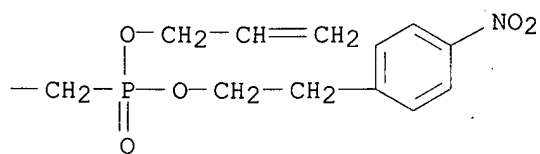


 — OMe

RN 185670-97-7 HCAPLUS

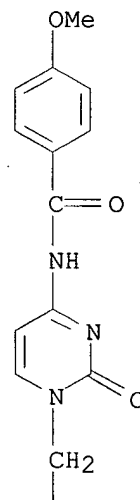
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[2-(4-nitrophenyl)ethoxy](2-propenyloxy)phosphinyl)methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)



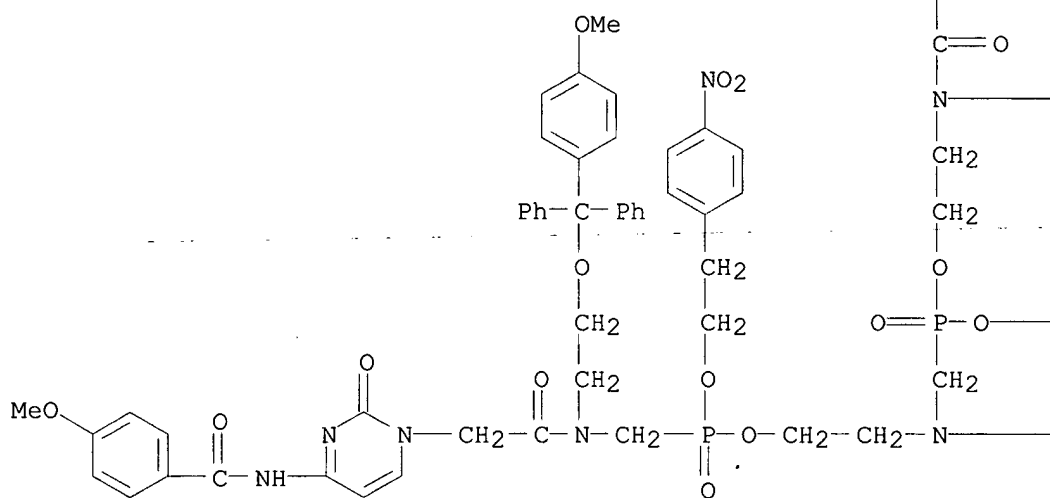


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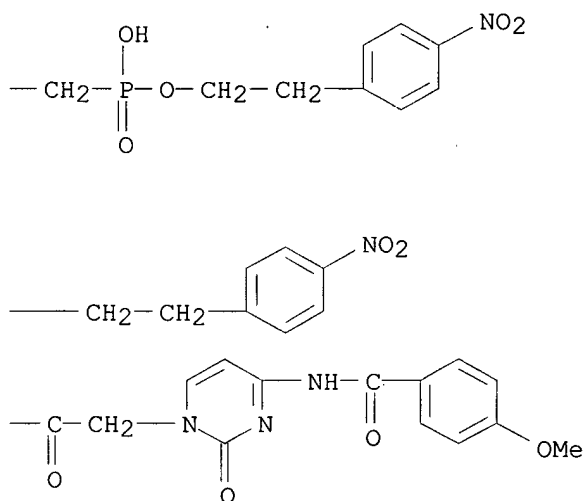
CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[hydroxy[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl][[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)



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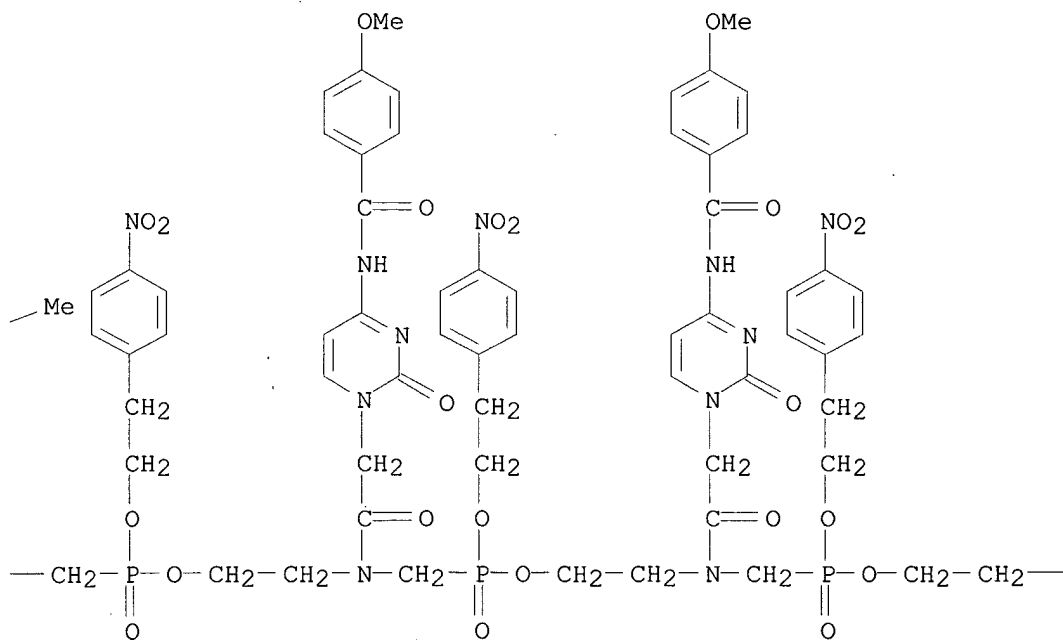
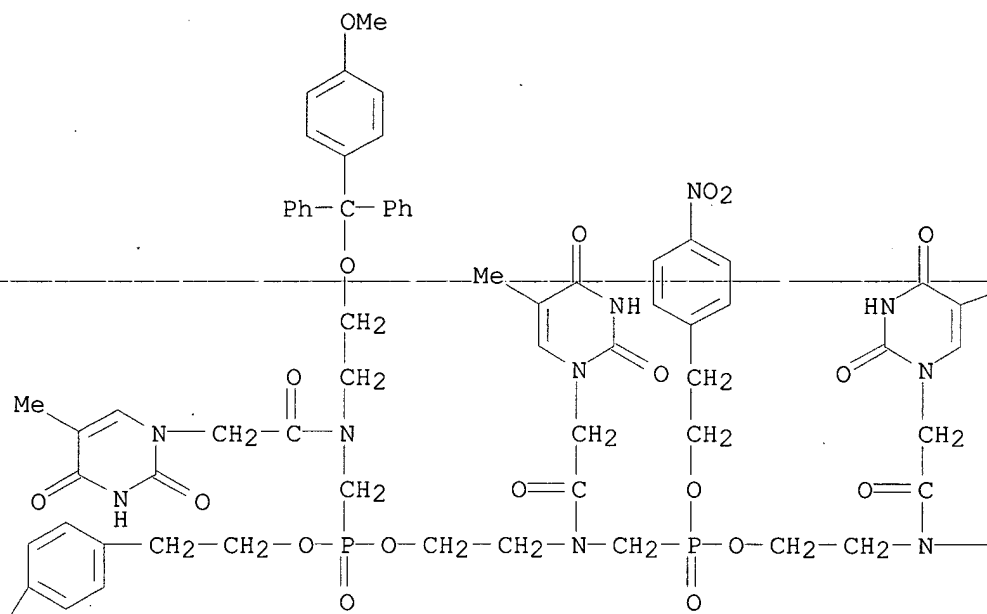


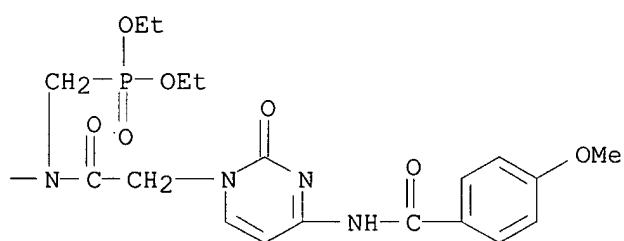
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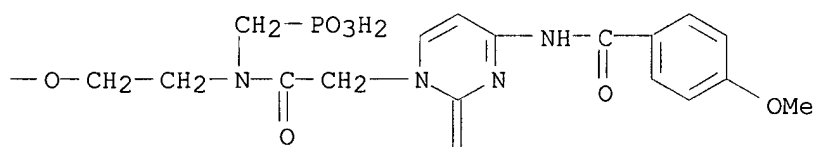
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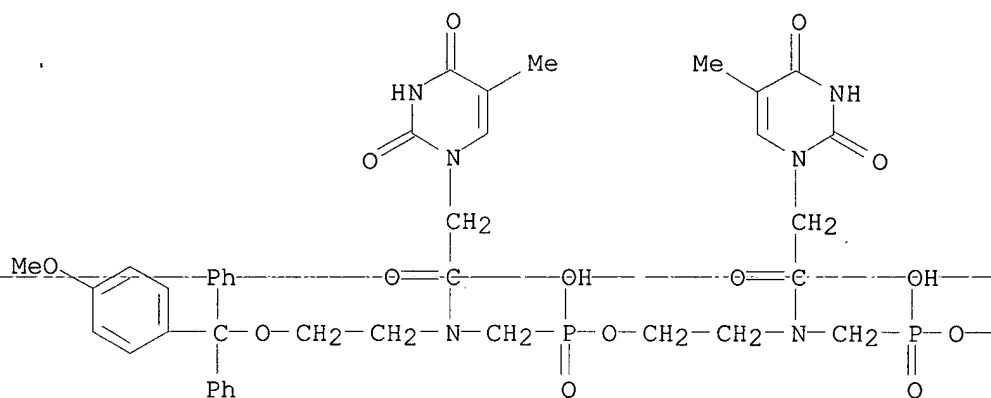
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RN 185671-00-5 HCAPLUS
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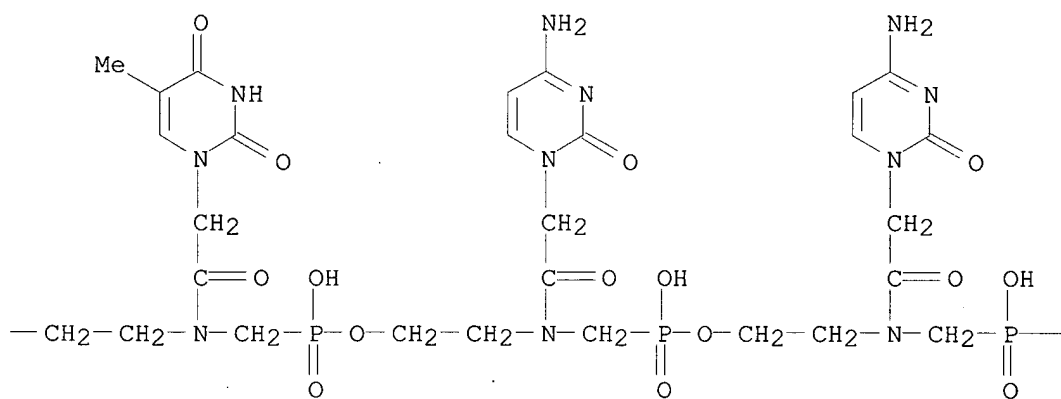


RN 185671-01-6 HCAPLUS
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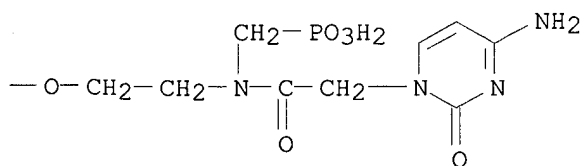
PAGE 1-A



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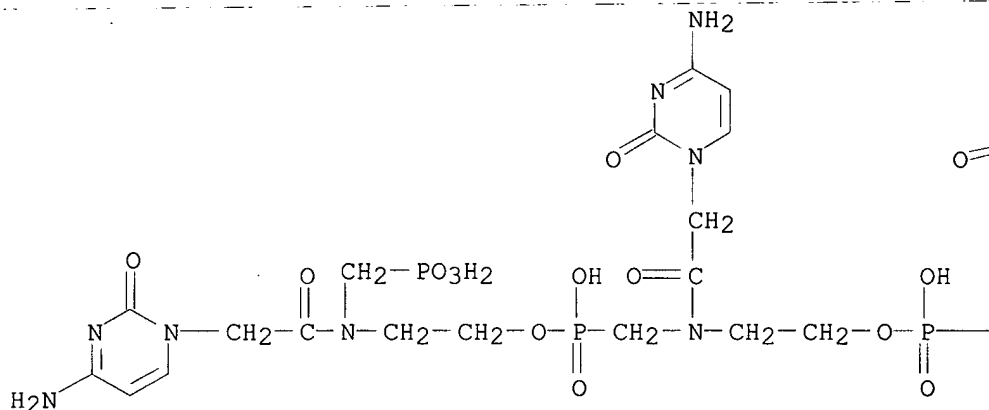
PAGE 1-C



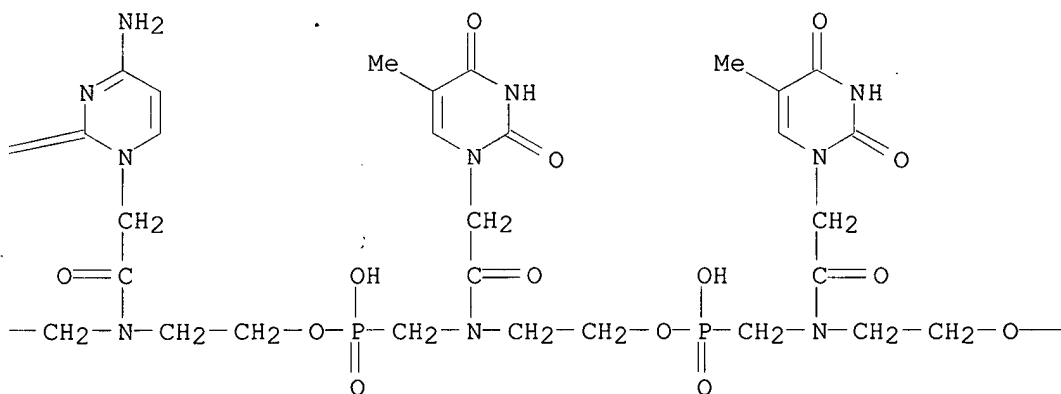
RN 185671-02-7 HCAPLUS

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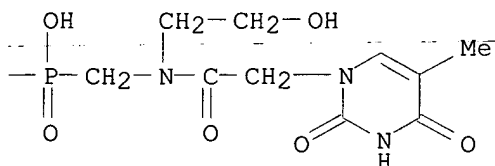
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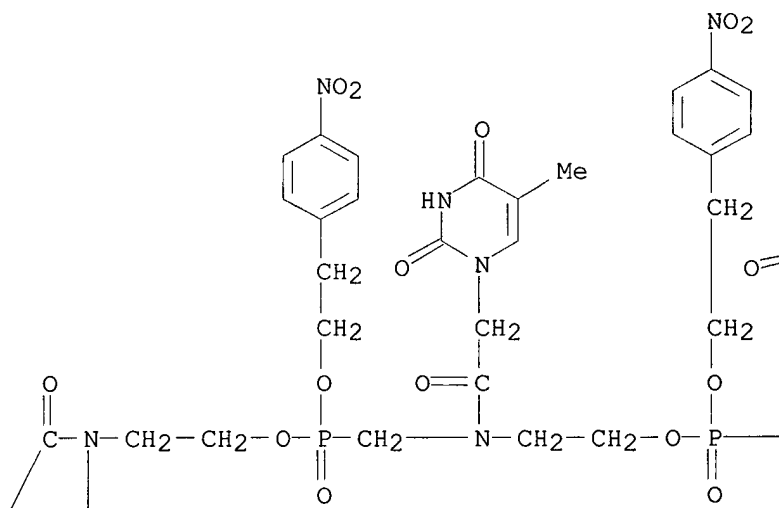
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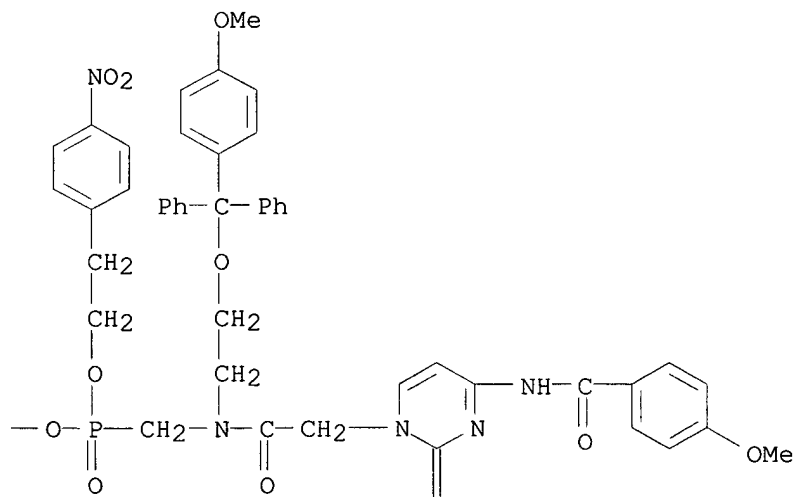
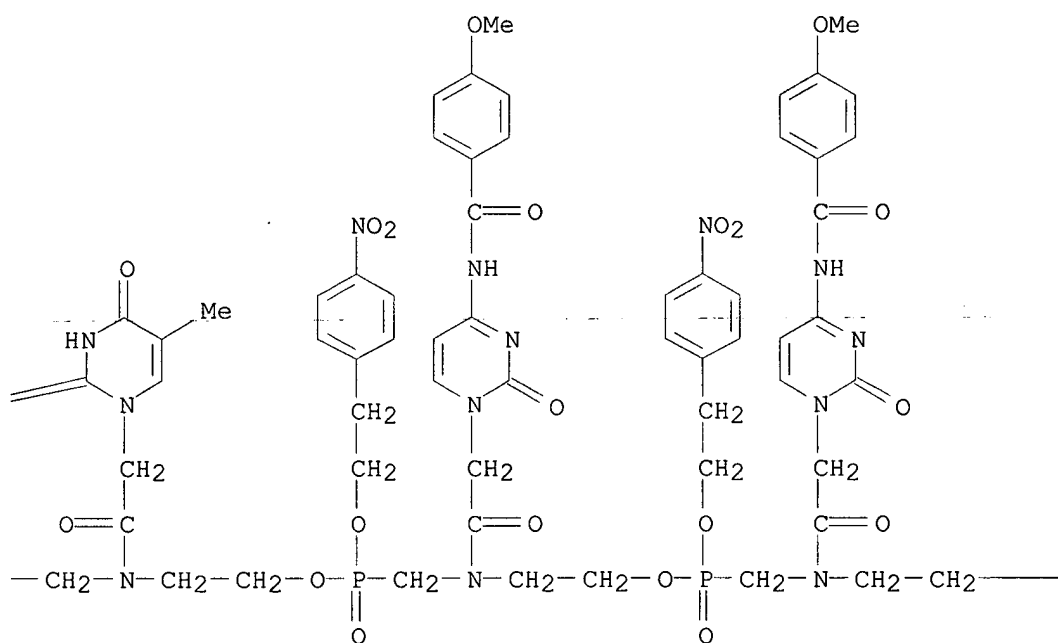


RN 185671-03-8 HCAPLUS

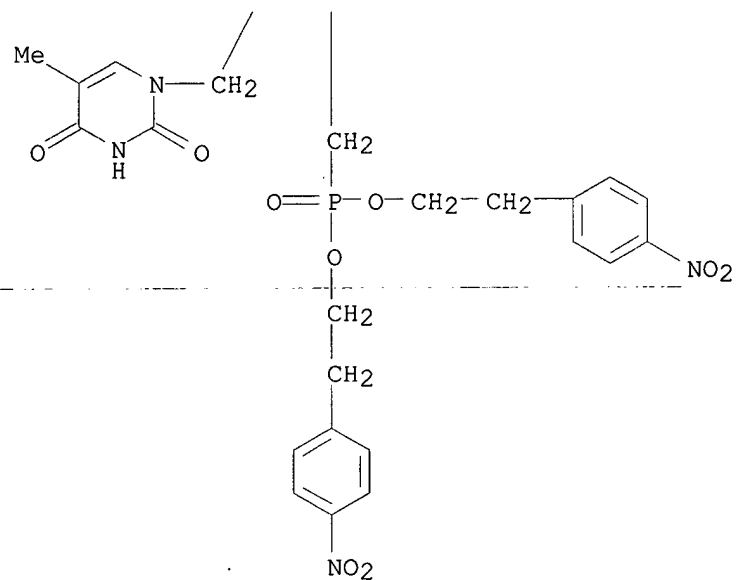
CN Phosphonic acid, [2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8,14,20-tris[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetetracos-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14-(4-nitrophenyl)-5,11-bis[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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L13 ANSWER 9 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:755989 HCAPLUS

DOCUMENT NUMBER: 126:118140

TITLE: Phosphonic ester nucleic acids (PHONAs):
oligodeoxyribonucleotide analog with an achiral
phosphonic acid ester backbone

AUTHOR(S): Peyman, Anusch; Uhlmann, Eugen; Wagner, Konrad;
Augustin, Sascha; Breipohl, Gerhard; Will, David W.;
Schaefer, Andrea; Wallmeier, Holger

~~CORPORATE SOURCE: Hoechst AG, Frankfurt, D-65926, Germany~~

SOURCE: Angewandte Chemie, International Edition in English
(1996), 35(22), 2636-2638
CODEN: ACIEAY; ISSN: 0570-0833

PUBLISHER: VCH

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The prepn. of polyamide nucleic acid analogs with an achiral and neg.
charged backbone to which the nucleobases are attached through
carboxymethylene linkers, is reported.

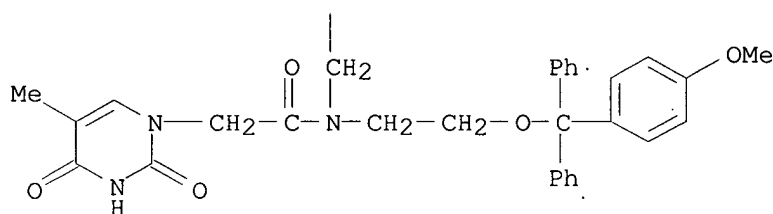
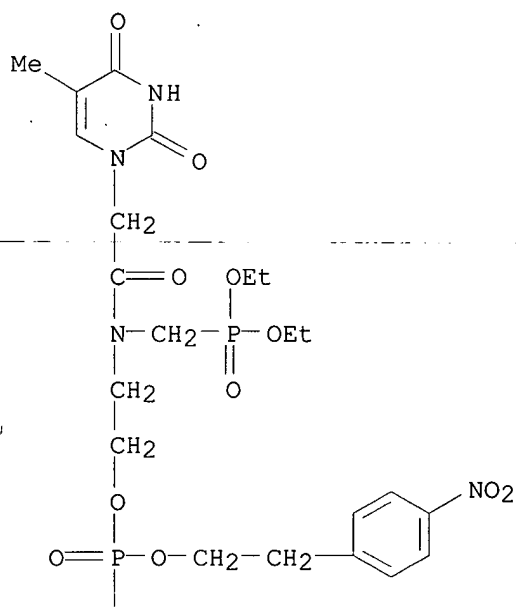
IT 183058-04-0P 183058-10-8P 185670-60-4P
185670-64-8P 185670-74-0P 186143-35-1P
186143-36-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(prepn. of phosphonic ester nucleic acid duplexes)

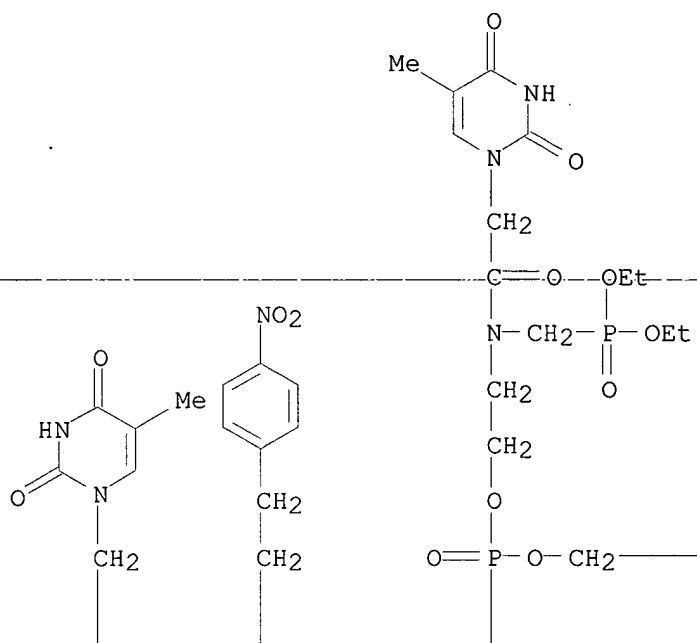
RN 183058-04-0 HCAPLUS

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pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-
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ester (9CI) (CA INDEX NAME)

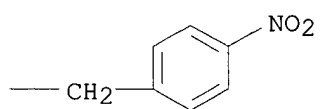


RN 183058-10-8 HCAPLUS
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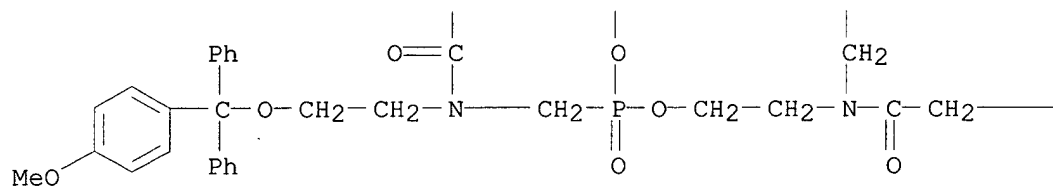
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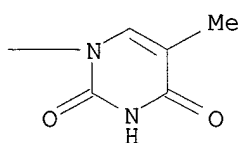
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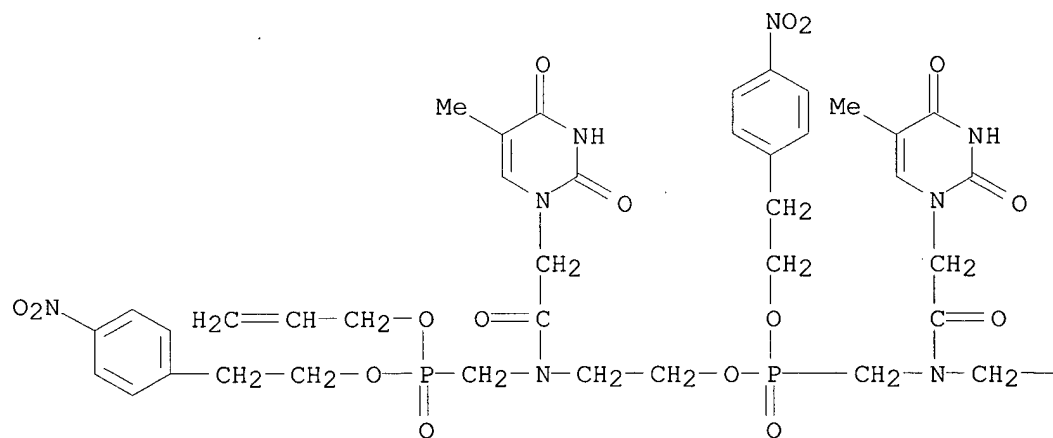
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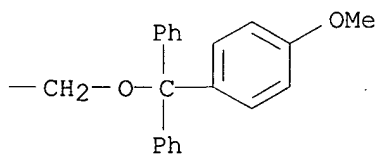


RN 185670-60-4 HCAPLUS

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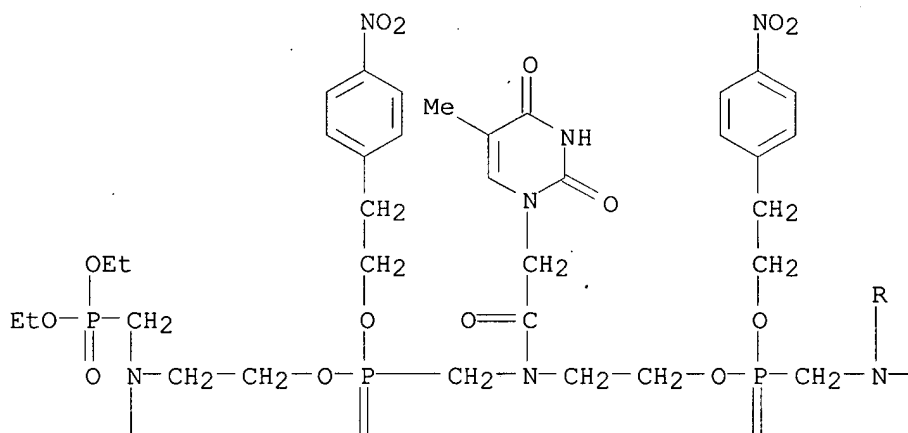
PAGE 1-A



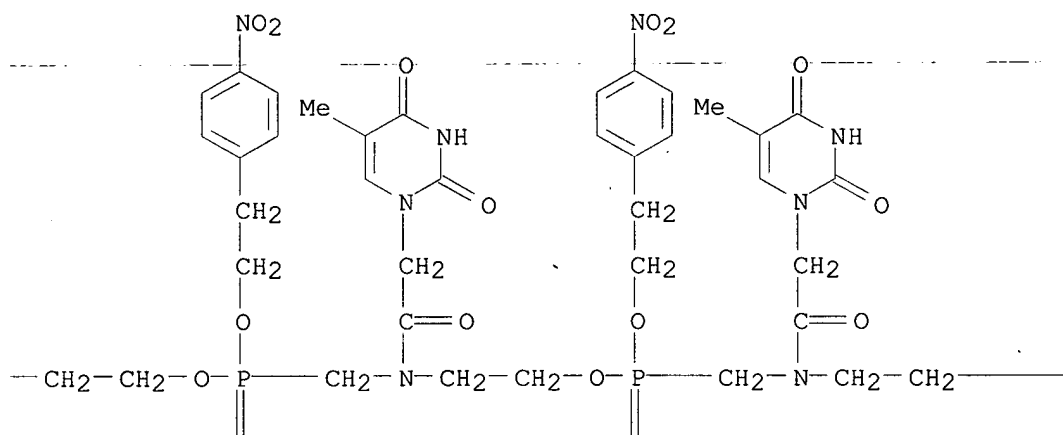


RN 185670-64-8. HCAPLUS

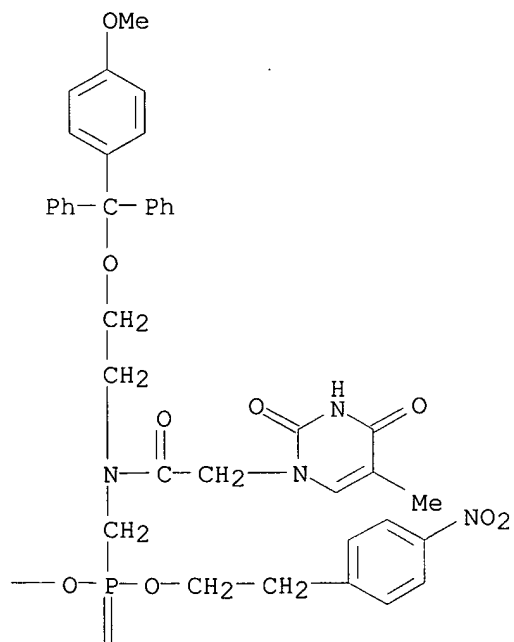
CN Phosphonic acid, [2,8,14,20-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-24-(4-methoxyphenyl)-6,12,18-tris[2-(4-nitrophenyl)ethoxy]-6,12,18-trioxido-24,24-diphenyl-5,11,17,23-tetraoxa-2,8,14,20-tetraaza-6,12,18-triphosphatetetracos-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)



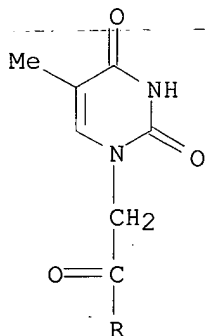
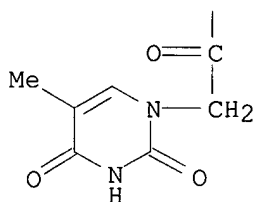
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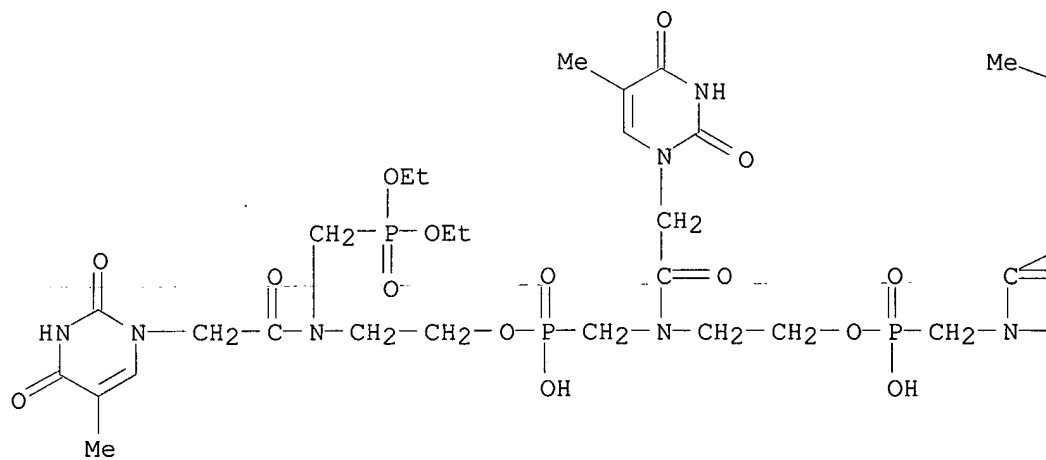


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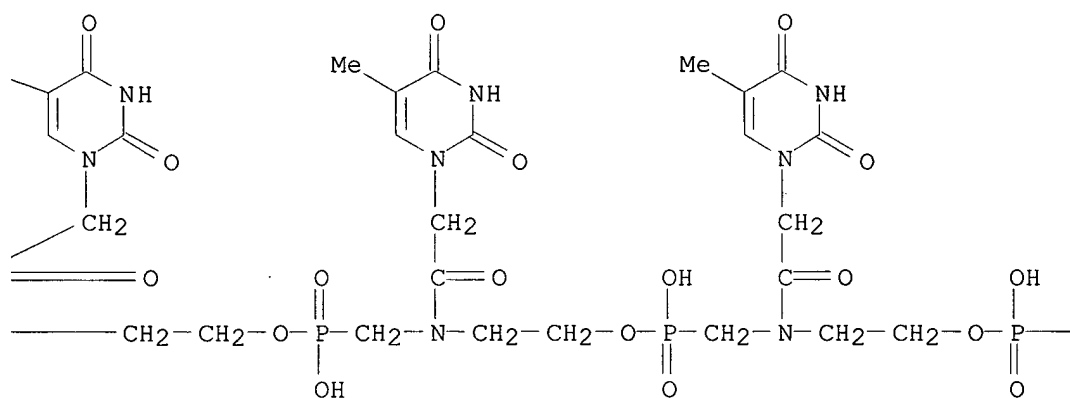


RN 185670-74-0 HCAPLUS
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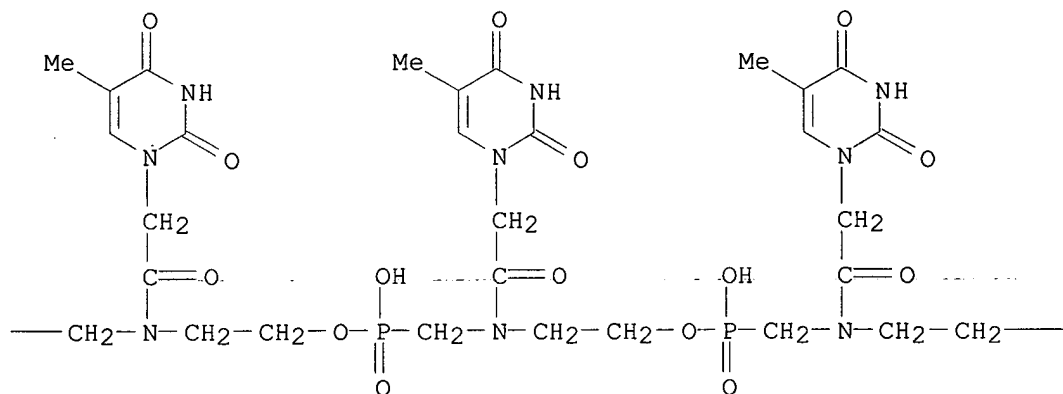
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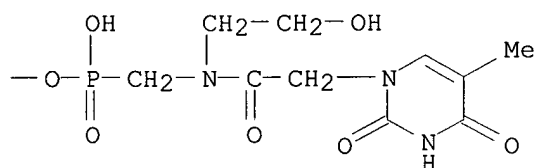
PAGE 1-B



PAGE 1-C

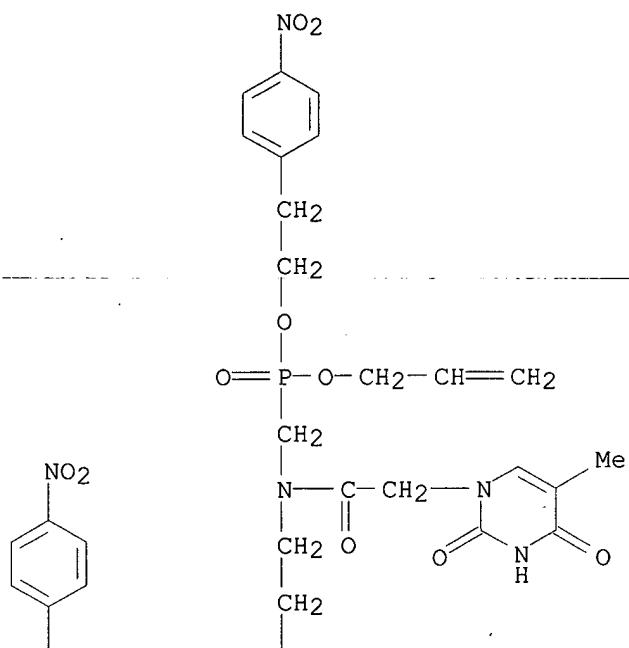


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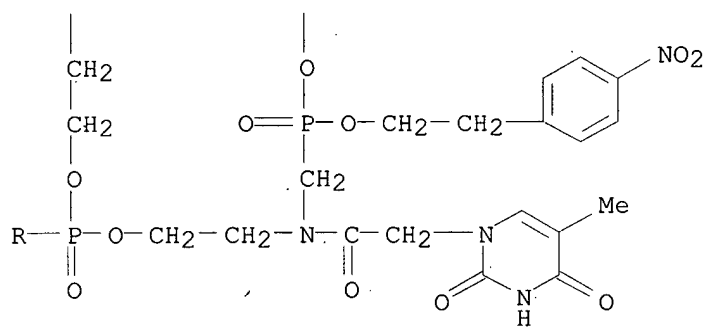


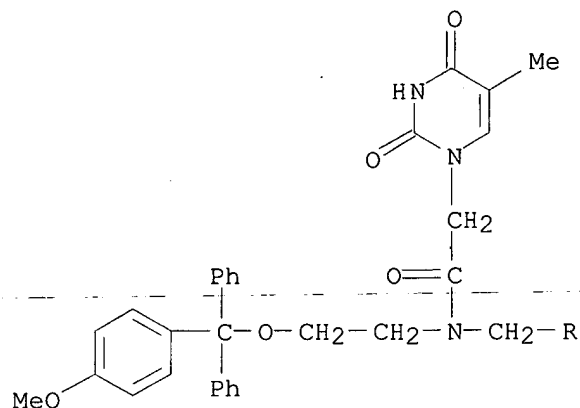
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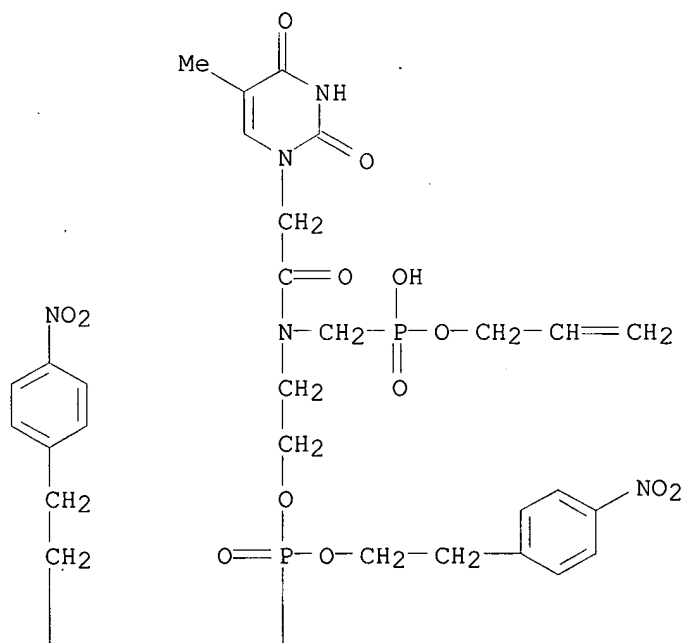


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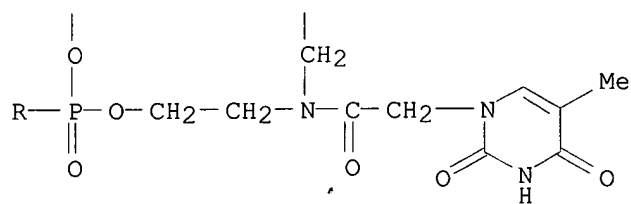




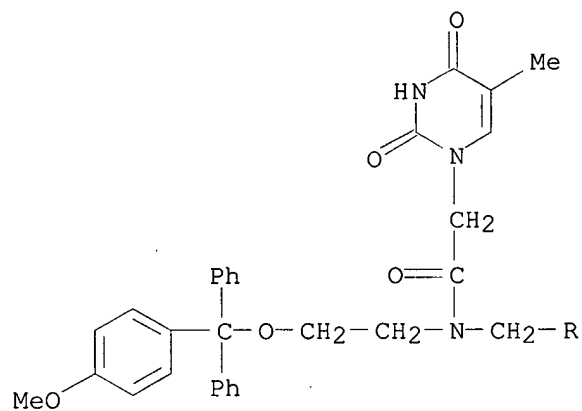
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L13 ANSWER 10 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:672510 HCAPLUS

DOCUMENT NUMBER: 125:301493

TITLE: Preparation of nucleic acid phosphonoesters as inhibitors of gene expression.

INVENTOR(S): Anuschirwan, Peyman; Uhlmann, Eugen; Breipohl, Gerhard; Wallmeier, Holger

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Ger. Offen., 36 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19508923	A1	19960919	DE 1995-19508923	19950313
EP 739898	A2	19961030	EP 1996-103533	19960307
EP 739898	A3	19980916		
EP 739898	B1	20010926		
R: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE				
AT 206131	E	20011015	AT 1996-103533	19960307
US 5874553	A	19990223	US 1996-613417	19960311
CA 2171589	AA	19960914	CA 1996-2171589	19960312
NO 9601006	A	19960916	NO 1996-1006	19960312
AU 9648028	A1	19960926	AU 1996-48028	19960312
AU 706470	B2	19990617		
ZA 9601986	A	19961121	ZA 1996-1986	19960312
BR 9600993	A	19971230	BR 1996-993	19960312
JP 08259579	A2	19961008	JP 1996-84808	19960313
CN 1138588	A	19961225	CN 1996-100508	19960313
CN 1060781	B	20010117		
US 6127346	A	20001003	US 1998-196132	19981120

PRIORITY APPLN. INFO.:

DE 1995-19508923 A 19950313

DE 1995-19543865 A 19951124

US 1996-613417 A1 19960311

AB QXP(Z)(:Y)CR5R6L(AB)DGX[P(Z)(:Y)CR5R6L(AB)DGX]nQ1 [n = 0-100; B = H, OH, alkoxy, alkylthio, (un)natural nucleobase, reporter ligand, (substituted) alkyl, aryl, aralkyl, heterocyclyl, etc.; AB = amino acid or peptide residue; R1 = H, (substituted) alkyl; R5, R6 = H, (substituted) alkyl, aryl, aralkyl, OH, alkoxy, alkylthio; A = bond, CH2, (O-, S-, or NR1-interrupted) (substituted) alkylene; D, G = (substituted) methylene; X, Y = O, S, NR1; Z = OH, alkoxy, alkenyloxy, alkynyloxy, amino, etc.; Q, Q1 = H, conjugate, (modified) oligonucleotide], were prepd. as drugs and diagnostic agents (no data). Thus, N-(4-methoxytriphenylmethoxy)ethylaminomethanephosphonic acid di[2-(p-nitrophenyl)ethyl]ester (prepn. given) was stirred with N-ethylmorpholine, HATU, and N6-anisoylcytosine-1-acetic acid in DMF to give a coupling product which was stirred with DBU in MeCN to give N-(N6-anisoylcytosine-1-ylacetyl)-N-(4-methoxytriphenylmethoxy)ethylaminomethanephosphonic acid [2-(p-nitrophenyl)ethyl] monoester.

IT 183057-63-8P 183057-66-1P 183057-94-5P

183058-06-2P 183058-10-8P 183058-11-9P

183058-12-0P 183058-14-2P

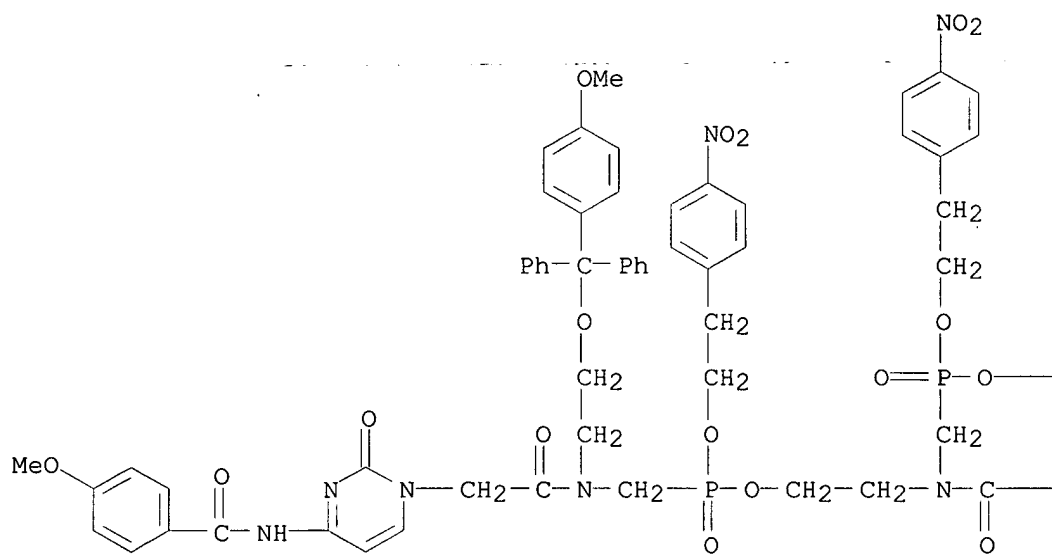
RL: BAC (Biological activity or effector, except adverse); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of nucleic acid phosphonoesters as inhibitors of gene expression)

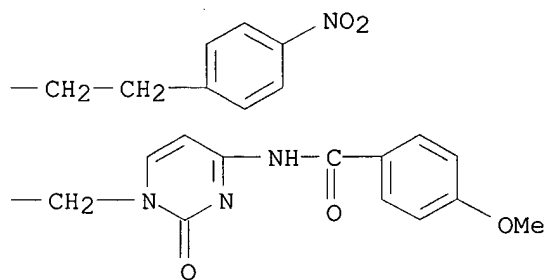
RN 183057-63-8 HCAPLUS

CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, bis[2-(4-nitrophenyl)ethyl] ester (9CI) (CA INDEX NAME)

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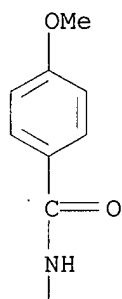
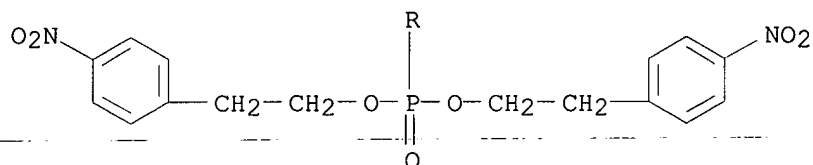
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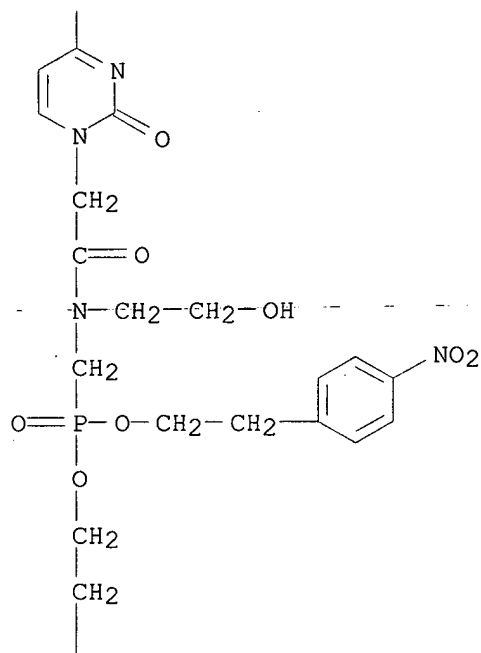
RN 183057-66-1 HCAPLUS

CN Phosphonic acid, [[(2-hydroxyethyl)[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]methyl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

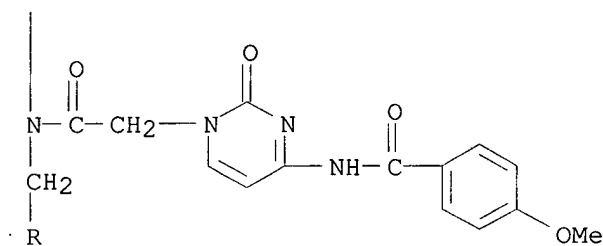
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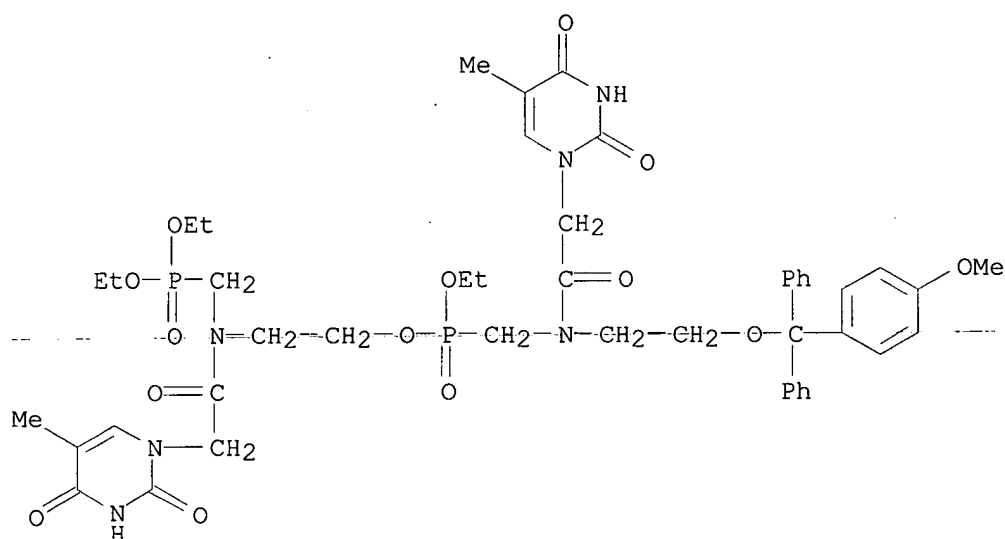
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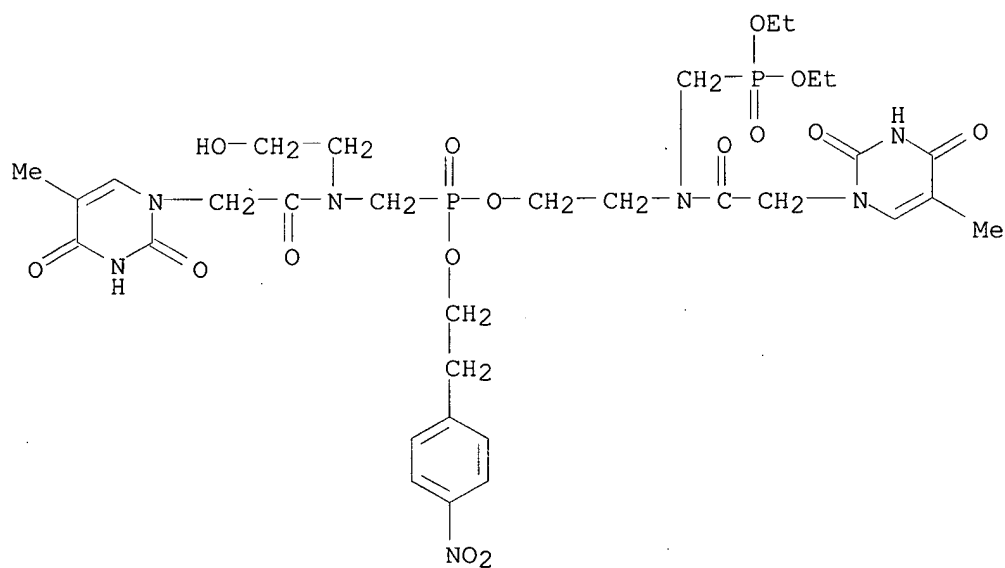


RN 183057-94-5 HCAPLUS
 CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-6-ethoxy-12-(4-methoxyphenyl)-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)



RN 183058-06-2 HCAPLUS

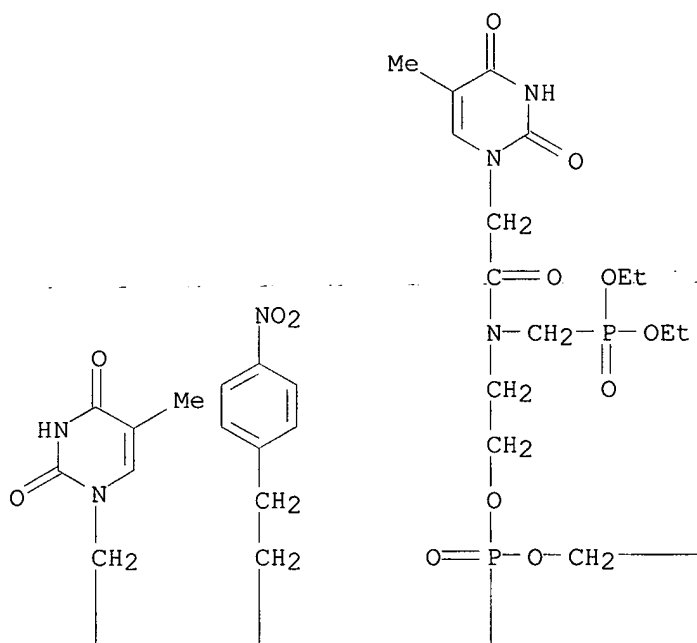
CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)



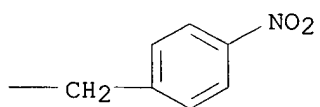
RN 183058-10-8 HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

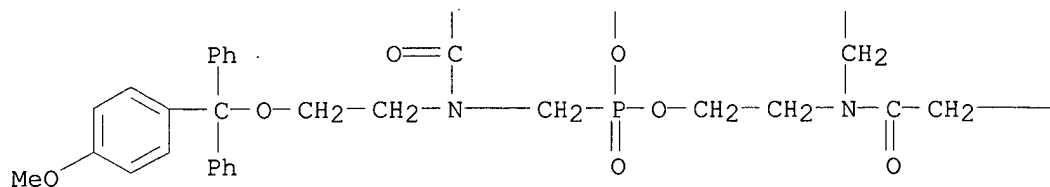
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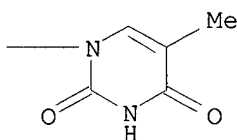
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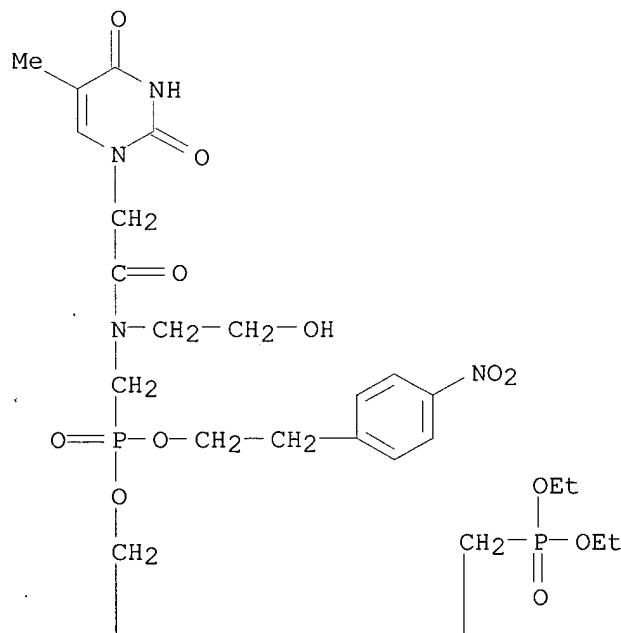
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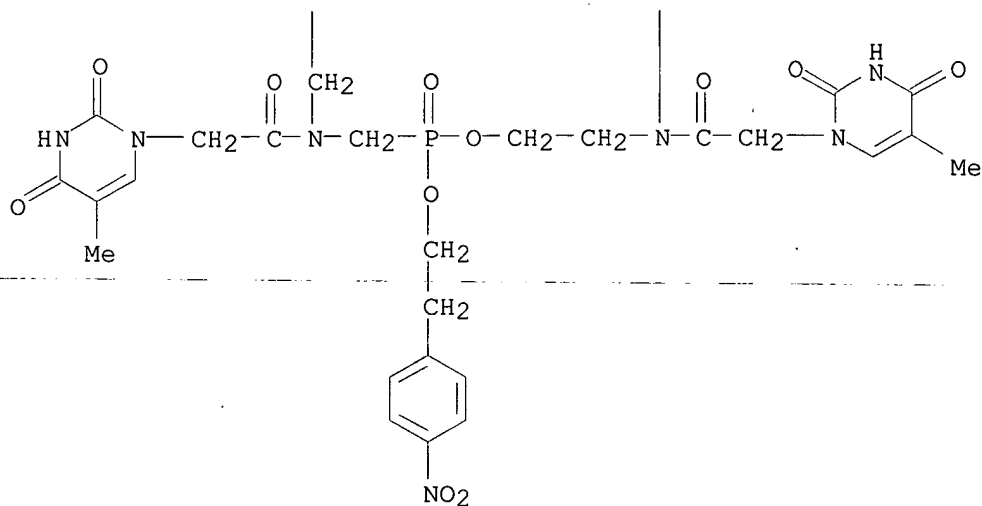
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CN Phosphonic acid, [10-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2-[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-8-(2-hydroxyethyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-9-oxo-5-oxa-2,8-diaza-6-phosphadec-1-yl]-, 2-[[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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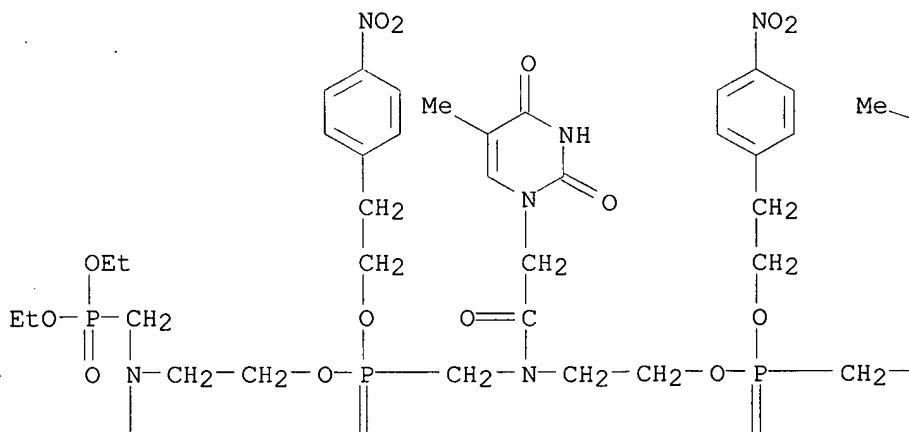
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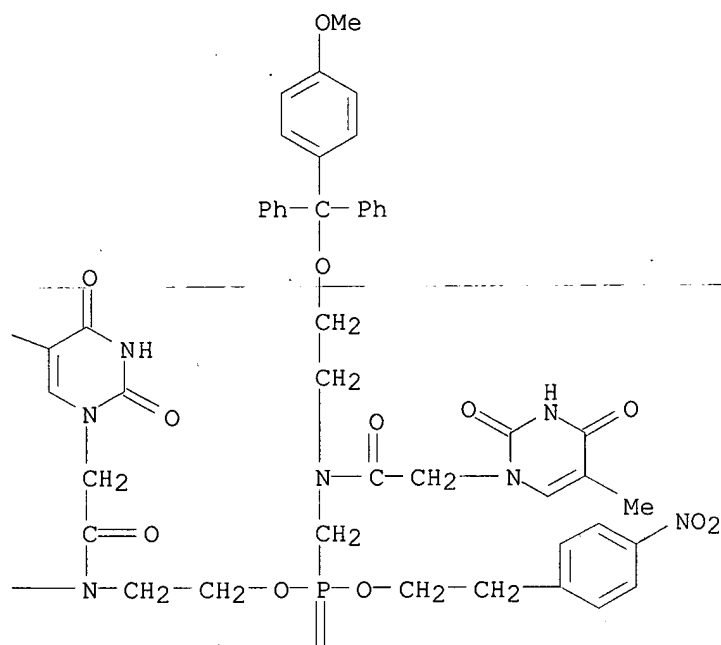
RN 183058-12-0 HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, 3,9-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-11-ethoxy-5-[2-(4-nitrophenyl)ethoxy]-5,11-dioxido-6,12-dioxa-3,9-diaza-5,11-diphosphatetradec-1-yl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

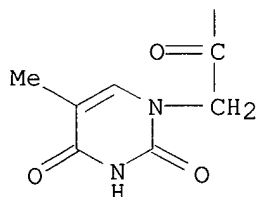
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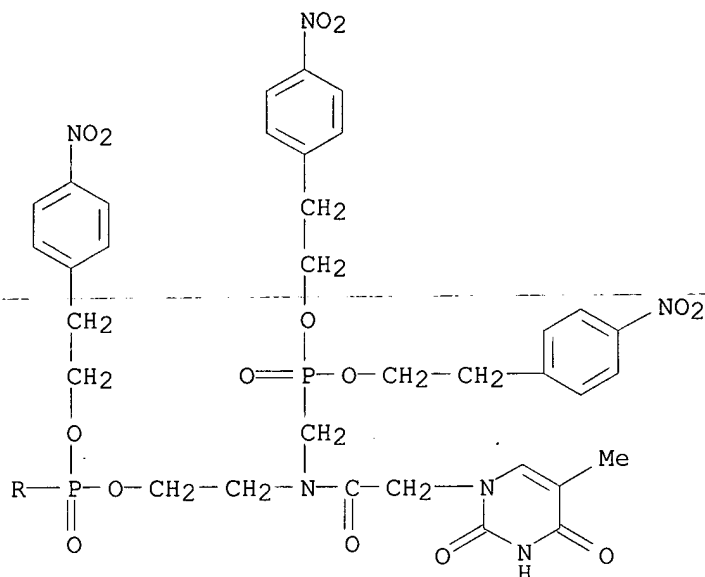


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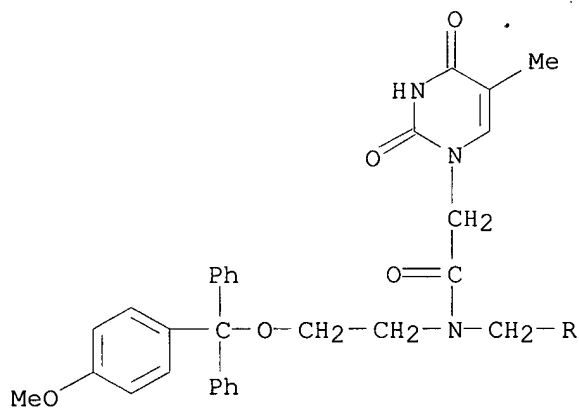


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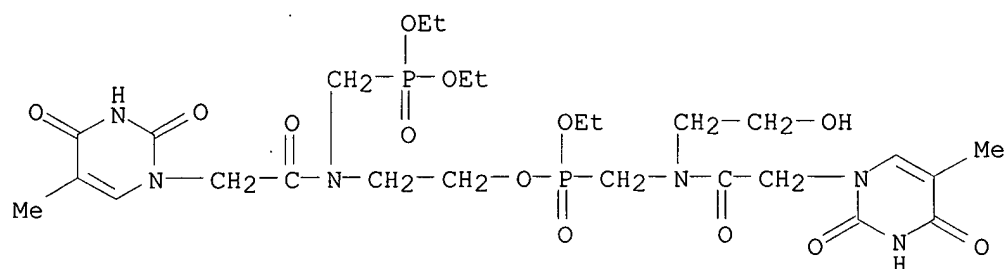
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 183058-09-5P 183058-13-1P 183058-15-3P
 183058-16-4P 183058-18-6P

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of nucleic acid phosphonoesters as inhibitors of gene expression)

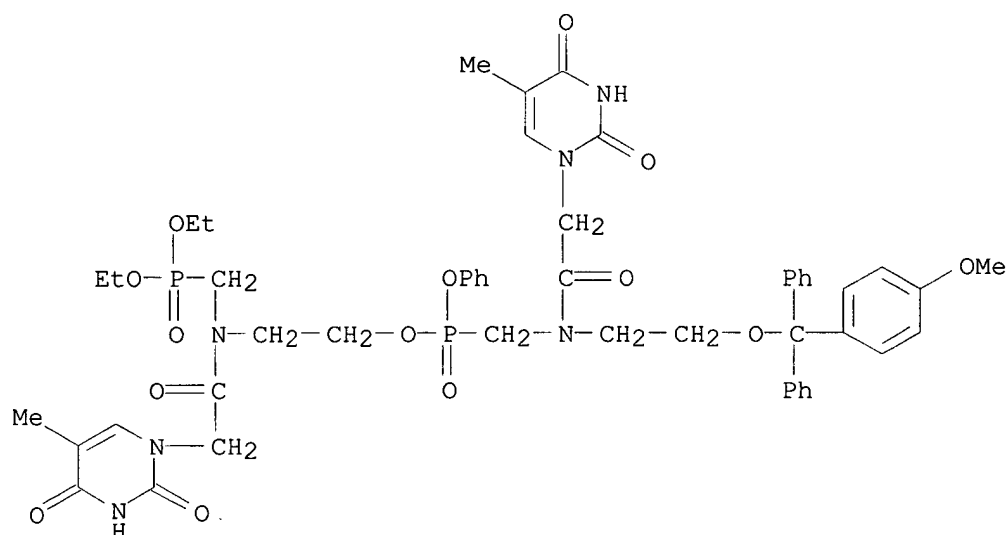
RN 183057-96-7 HCAPLUS

CN Phosphonic acid, [[[3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl]acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl ethyl ester (9CI) (CA INDEX NAME)



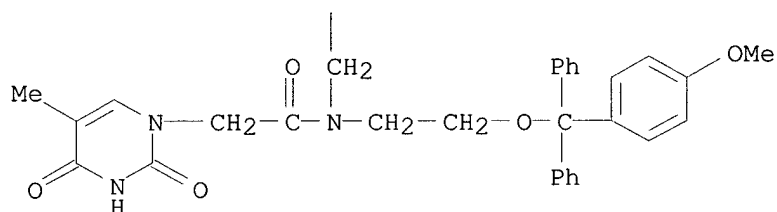
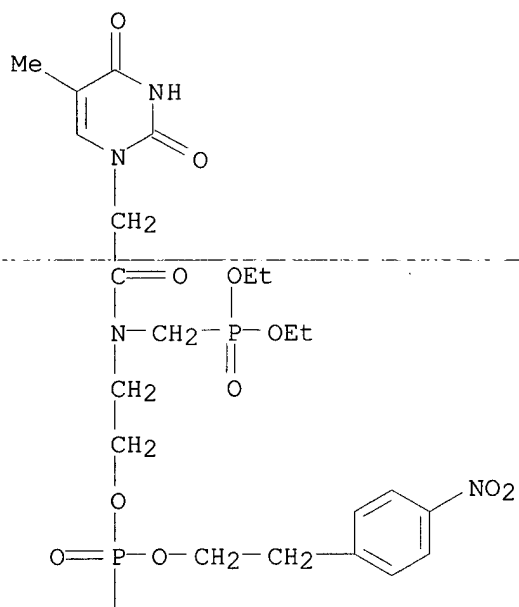
RN 183057-99-0 HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-oxido-6-phenoxy-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)



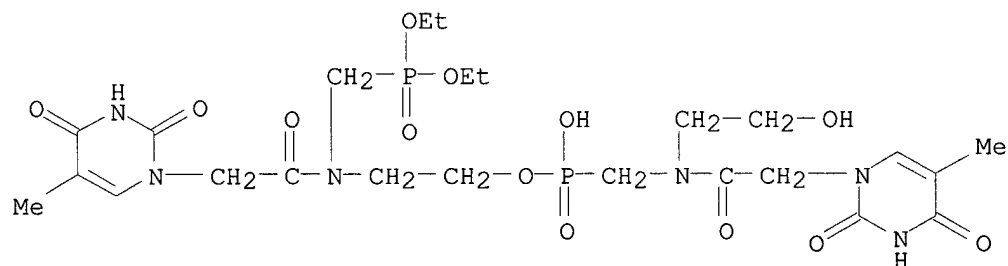
RN 183058-04-0 HCAPLUS

CN Phosphonic acid, [2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxa-2,8-diaza-6-phosphadodec-1-yl]-, diethyl ester (9CI) (CA INDEX NAME)



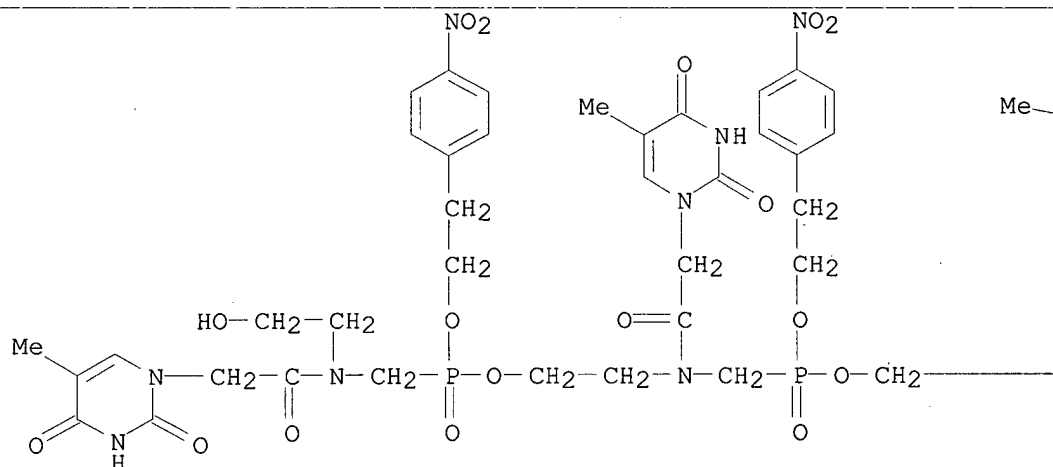
RN 183058-09-5 HCAPLUS

CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl] (2-hydroxyethyl)amino]methyl]-, mono[2-[[[(diethoxyphosphinyl)methyl] [(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl] ester (9CI) (CA INDEX NAME)

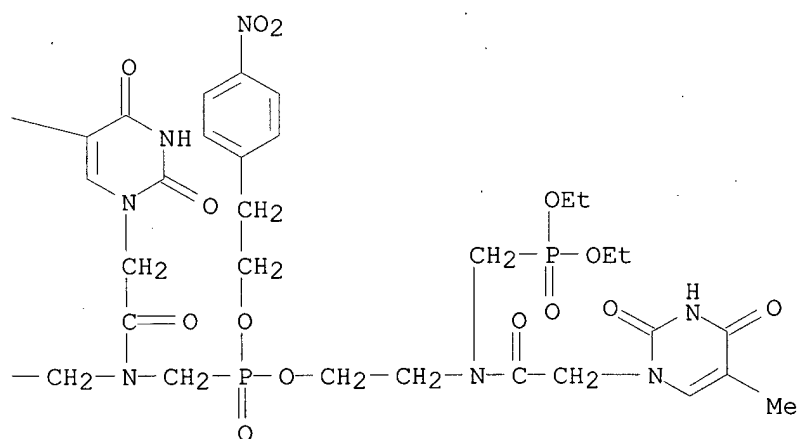


RN 183058-13-1 HCAPLUS
 CN Phosphonic acid, [16-(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)-2,8-bis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-14-(2-hydroxyethyl)-6,12-bis[(4-nitrophenyl)ethoxy]-6,12-dioxido-15-oxo-5,11-dioxo-2,8,14-triaza-6,12-diphosphahexadec-1-yl]-, 2-[[[(diethoxyphosphinyl)methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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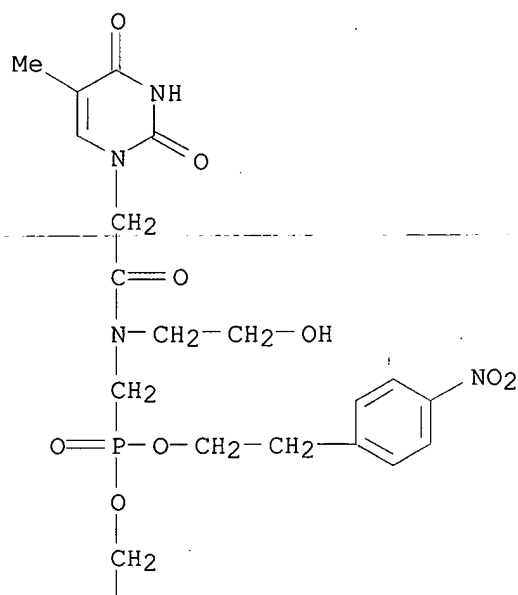


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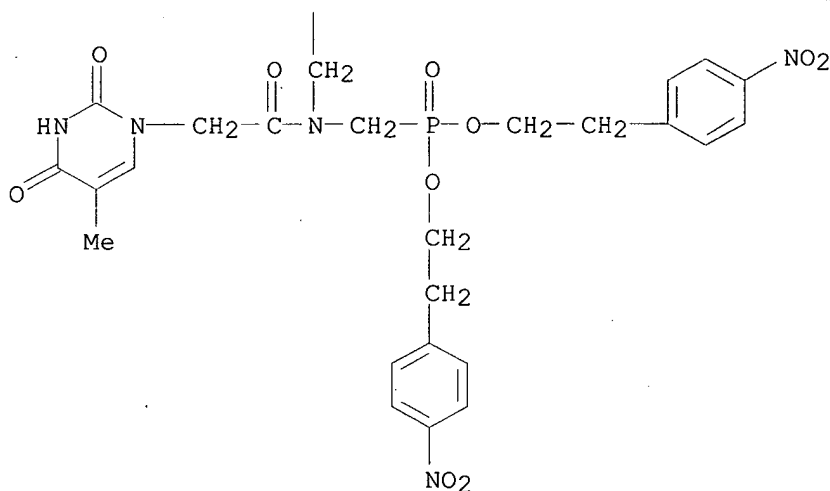


RN 183058-15-3 HCAPLUS
 CN Phosphonic acid, [[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl](2-hydroxyethyl)amino]methyl]-, 2-[[[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl][(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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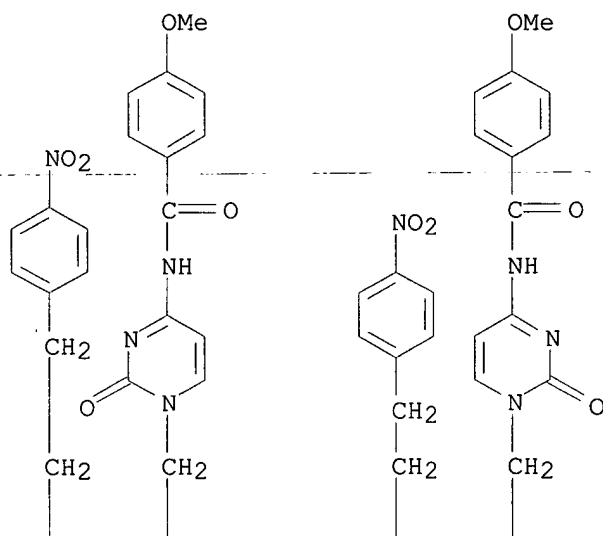


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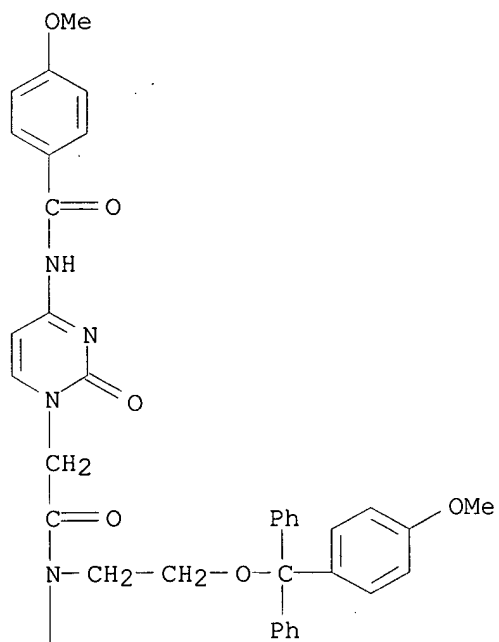


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 CN Phosphonic acid, [2,8-bis[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-12-(4-methoxyphenyl)-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-12,12-diphenyl-5,11-dioxo-2,8-diaza-6-phosphadodec-1-yl]-, 2-[[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl][[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

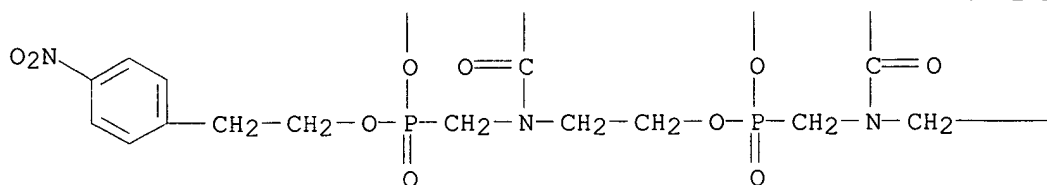
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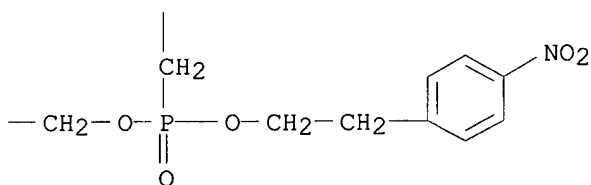
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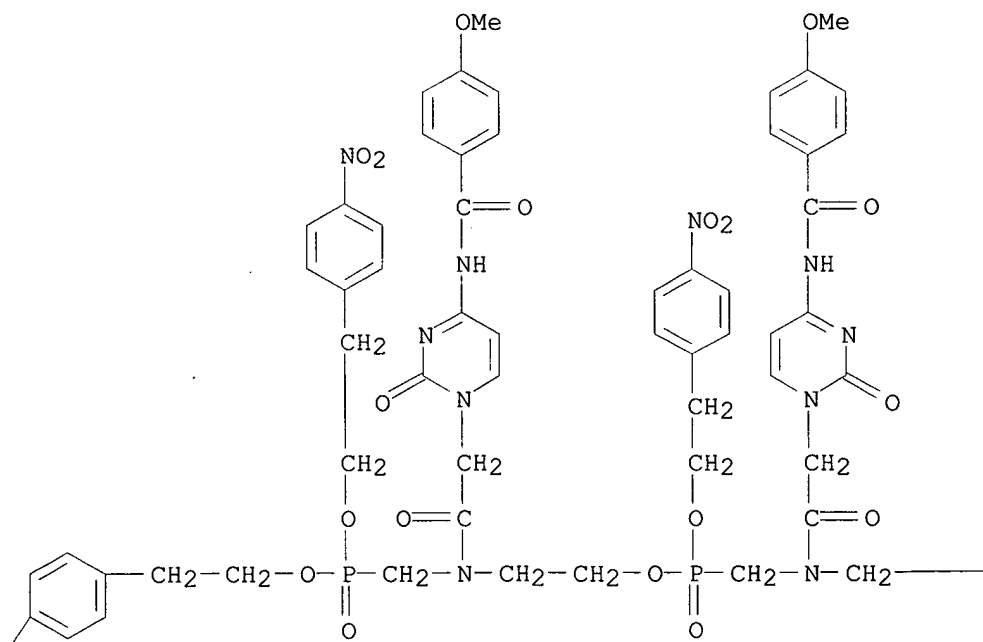


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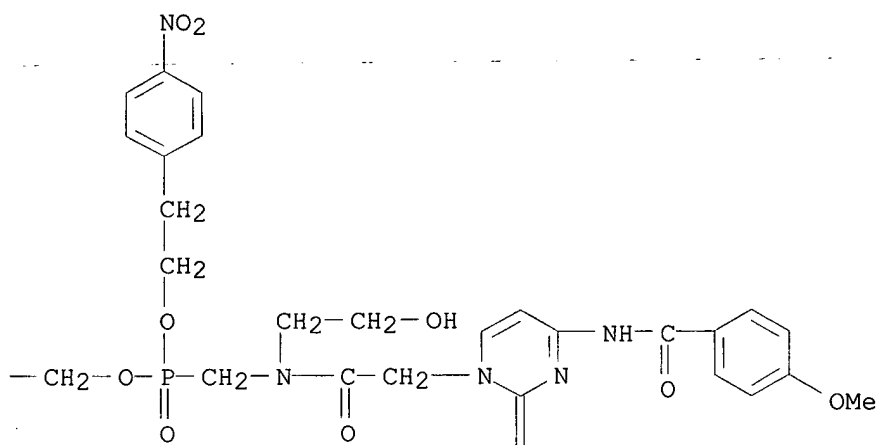


RN 183058-18-6 HCAPLUS
 CN Phosphonic acid, [8-(2-hydroxyethyl)-10-[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]-2-[[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]-6-[2-(4-nitrophenyl)ethoxy]-6-oxido-9-oxo-5-oxa-2,8-diaza-6-phosphadec-1-yl]-, 2-[[[bis[2-(4-nitrophenyl)ethoxy]phosphinyl]methyl][[4-[(4-methoxybenzoyl)amino]-2-oxo-1(2H)-pyrimidinyl]acetyl]amino]ethyl 2-(4-nitrophenyl)ethyl ester (9CI) (CA INDEX NAME)

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L13 ANSWER 11 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:55156 HCAPLUS

DOCUMENT NUMBER: 124:218502

TITLE: Extent of hydration of octadentate lanthanide complexes incorporating phosphinate donors: solution relaxometry and luminescence studies

AUTHOR(S): Aime, Silvio; Botta, Mauro; Parker, David; Williams, J. A. Gareth

CORPORATE SOURCE: Dip. Chim. Inorg., Univ. Torino, Turin, 10125, Italy

SOURCE: J. Chem. Soc., Dalton Trans. (1996), (1), 17-23

CODEN: JCDTBI; ISSN: 0300-9246

DOCUMENT TYPE: Journal

LANGUAGE: English

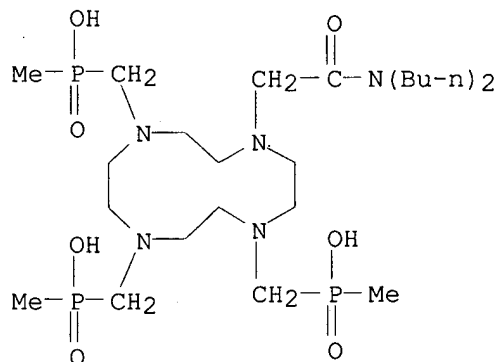
AB The behavior of luminescent (Eu, Tb) and highly paramagnetic (Gd) complexes of 1,4,7,10-tetraazacyclododecane contg. one carboxamide and three phosphinate substituents was studied in soln. Anal. of variable-temp. nuclear magnetic relaxation dispersion profiles indicate that there is no H₂O mol. directly coordinated to Gd(III) ions. The obsd. relaxation enhancement of solvent protons is detd., in addn. to the contribution from H₂O mols. diffusing in close proximity to the paramagnetic complex, by a relatively distant H₂O mol. in the 'second coordination sphere'. This is possible because the amide carbonyl O can participate in H bonding (as a H-bond acceptor) to a local H₂O mol., which brings the H₂O mol. close to the metal ion. The luminescence spectra of the complexes of Eu and Tb in H₂O and D₂O are also consistent with such a hydration scheme and there is a good correlation between the nonintegral q value (no. of inner-sphere H₂O mols.) detd. by this method and the distance between the metal ion and the H₂O proton estd. by relaxometric methods. Probably the hydration states q = 0 and 1 may be considered to represent boundary conditions and a given complex in soln. may possess intermediate values.

IT 145130-40-1P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(extent of hydration of octadentate lanthanide complexes incorporating phosphinate donors studied by soln. relaxometry and luminescence)

RN 145130-40-1 HCAPLUS

CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris(methyl- (9CI) (CA INDEX NAME)



MAUPIN 09/835,371

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L13 ANSWER 12 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:881296 HCAPLUS

DOCUMENT NUMBER: 123:286533

TITLE: Preparation of reagents comprising chimeric molecules of nucleic acids and nucleic acid analogs as primers

INVENTOR(S): Reeve, Michael Alan; Brown, Tom

PATENT ASSIGNEE(S): Amersham International PLC, UK

SOURCE: PCT Int. Appl., 39 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9476617	A1	19950410	AU 1994-76617	19940921
EP 720615	A1	19960710	EP 1994-927002	19940921
EP 720615	B1	20000726		
R: DE, DK, FR, GB, IT, SE				
US 2002068275	A1	20020606	US 1996-617781	19960521
PRIORITY APPLN. INFO.:			EP 1993-307455 A	19930921
			WO 1994-GB2053 W	19940921

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Chimeric mols. of nucleic acid/nucleic acid analog, comprising a nonstandard backboned oligonucleotide having at least one amide linkage and a std. backboned portion having a 3' acceptor end which is a chem. functionality capable of acting as an acceptor for the formation of a phosphodiester bond, useful as primers in reactions involving primer extension, such as nucleic acid amplification and sequencing, are prepd. A method for performing a primer extension reaction comprises mixing (a) a target nucleic acid (preferably a double-stranded nucleic acid), (b) a primer which is the said chimeric mol. capable of hybridizing to part of the target, and (c) a supply of nucleotides in the presence of a chain extension enzyme under conditions to allow the chimeric mol. to hybridize to the target and extension of the chimeric mol. at the acceptor end to occur and to give an extension product. A method for performing a chain termination reaction comprises mixing reagents a, b, and c (wherein preferably at least one of the reagents is labeled) in the presence of a chain extension enzyme under conditions to allow the chimeric mol. to hybridize to the target and extension of the chimeric mol. at the acceptor end to occur and to produce terminated extension products which are sepd. to allow part of the nucleotide sequence of the target nucleic acid to be detd. A method for detg. the nucleotide sequence of a target nucleic acid

comprises performing the latter method using a chain termination agent for each of the four different nucleotides such that the nucleotide sequence of the target may be detd. Thus, a peptide/oligonucleotide mol. (I) was prepd. by the solid phase method using std. phosphoramidite chem., a Applied Biosystems DNA synthesizer model 394, and intermediates Et N-(monomethoxytritylaminoethyl)-N-(thyminylacetyl)glycinate (II) (prepn. given) and 5'-amino-5'-deoxythymidine deriv. (III) (prepn. given). In primer extension assay using Klenow or exonuclease free Klenow, I gave efficient priming of the 18-mer DNA template 5'-CTGAACAACACTCTAAAA-3.

IT 169452-42-0P 169452-43-1P

RL: ARG (Analytical reagent use); BPR (Biological process); SPN (Synthetic preparation); ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); USES (Uses)

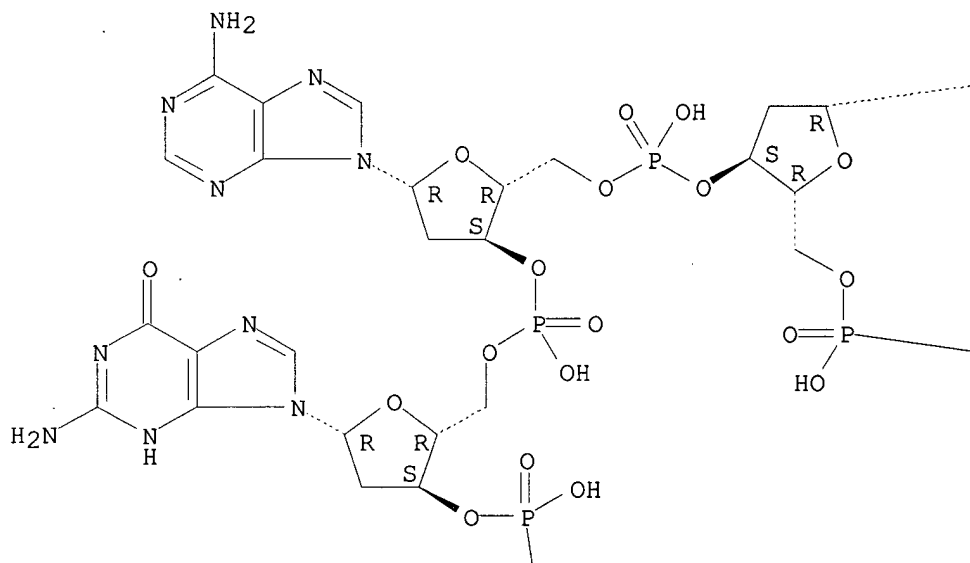
(prepn. of chimeric peptide/nucleic acid analogs contg. amide bonds as primers for DNA sequencing and amplification)

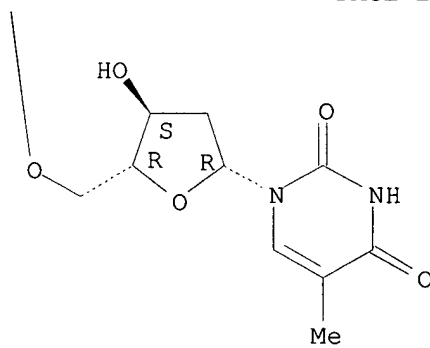
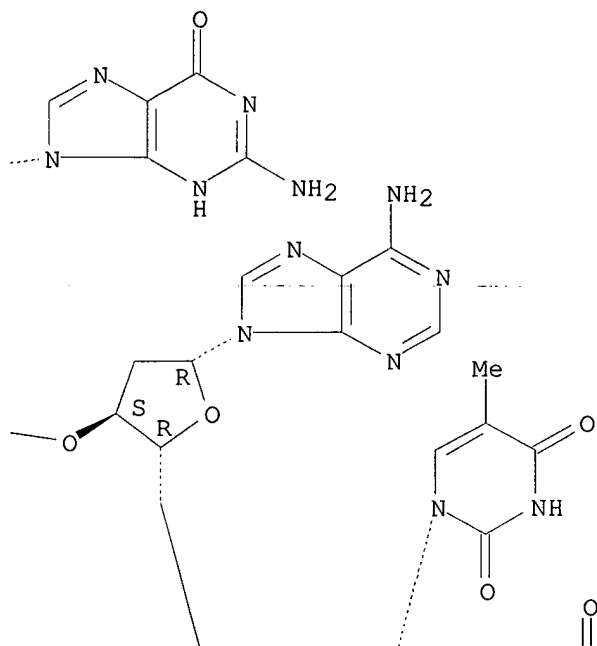
RN 169452-42-0 HCAPLUS

CN Thymidine, 5'-[[17-amino-3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13-trioxo-3,6,9,12,15-pentaazaheptadec-1-yl]amino]-5'-deoxythymidyl-(3'.fwdarw.5')-2'-deoxyadenyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2'-deoxyadenyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-(9CI) (CA INDEX NAME)

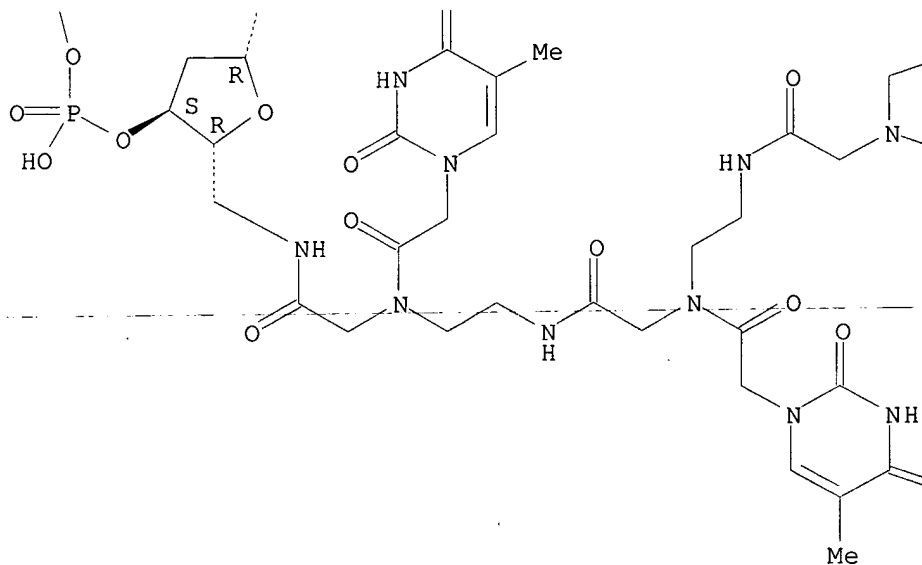
Absolute stereochemistry.

PAGE 1-A

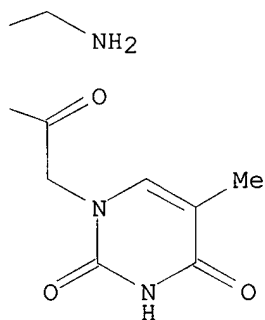




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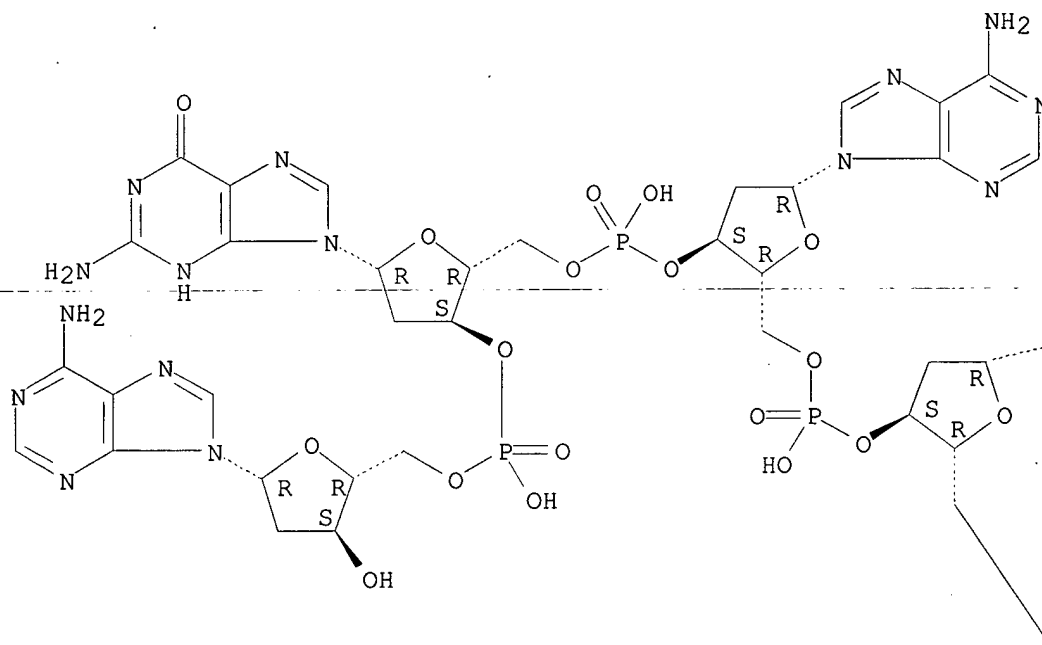


RN 169452-43-1 HCAPLUS

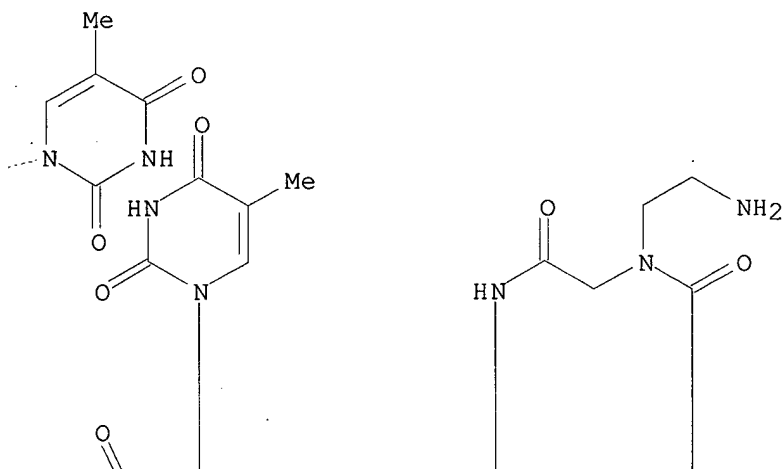
CN Adenosine, 5'-[[17-amino-3,9,15-tris[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13-trioxo-3,6,9,12,15-pentaazaheptadec-1-yl]amino]-5'-deoxythymidyl-(3'.fwdarw.5')-2'-deoxyadenyl-(3'.fwdarw.5')-2'-deoxyguanylyl-(3'.fwdarw.5')-2'-deoxy- (9CI) (CA INDEX NAME)

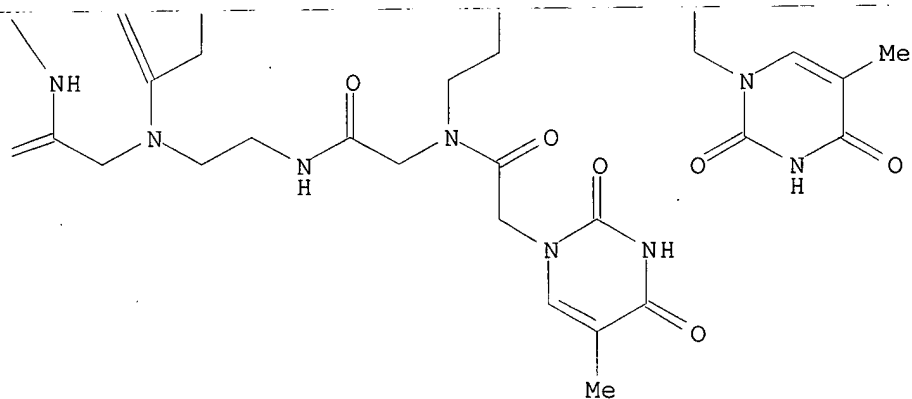
Absolute stereochemistry.

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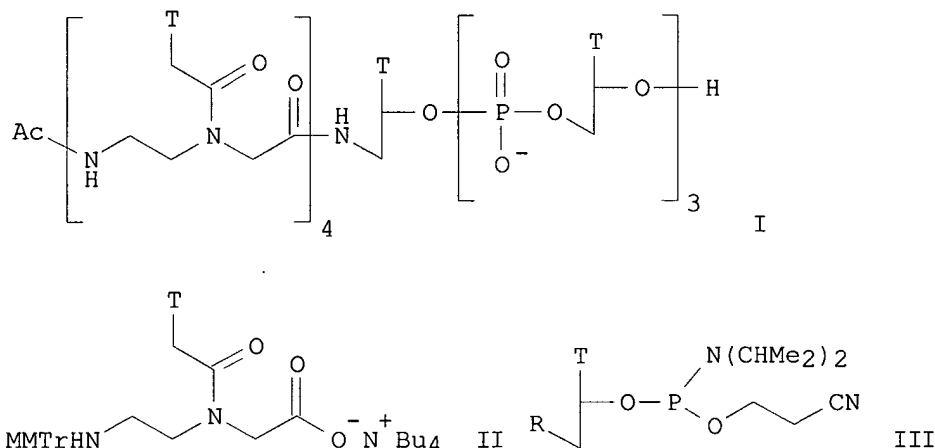
PAGE 1-B





=> d ibib abs hitstr 13

L13 ANSWER 13 OF 15 HCAPLUS COPYRIGHT 2002 ACS
 ACCESSION NUMBER: 1995:752363 HCAPLUS
 DOCUMENT NUMBER: 124:9293
 TITLE: Solid support synthesis of a PNA-DNA hybrid
 AUTHOR(S): van der Laan, A. C.; Meeuwenoord, N. J.;
 Kuyt-Yeheskiely, E.; Oosting, R. S.; Brands, R.; van
 Boom, J. H.
 CORPORATE SOURCE: Leiden Inst. Chem., Leiden Univ., Leiden, 2300 RA,
 Neth.
 SOURCE: Recl. Trav. Chim. Pays-Bas (1995), 114(6), 295-7
 CODEN: RTCPA3; ISSN: 0165-0513
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 GI



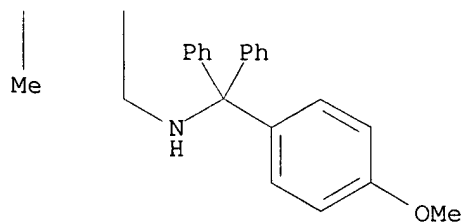
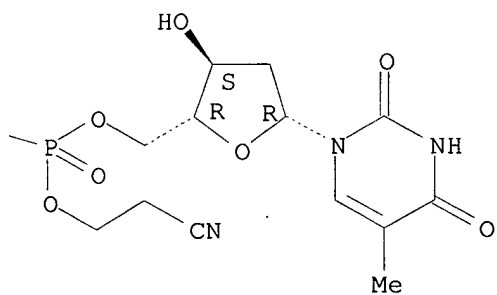
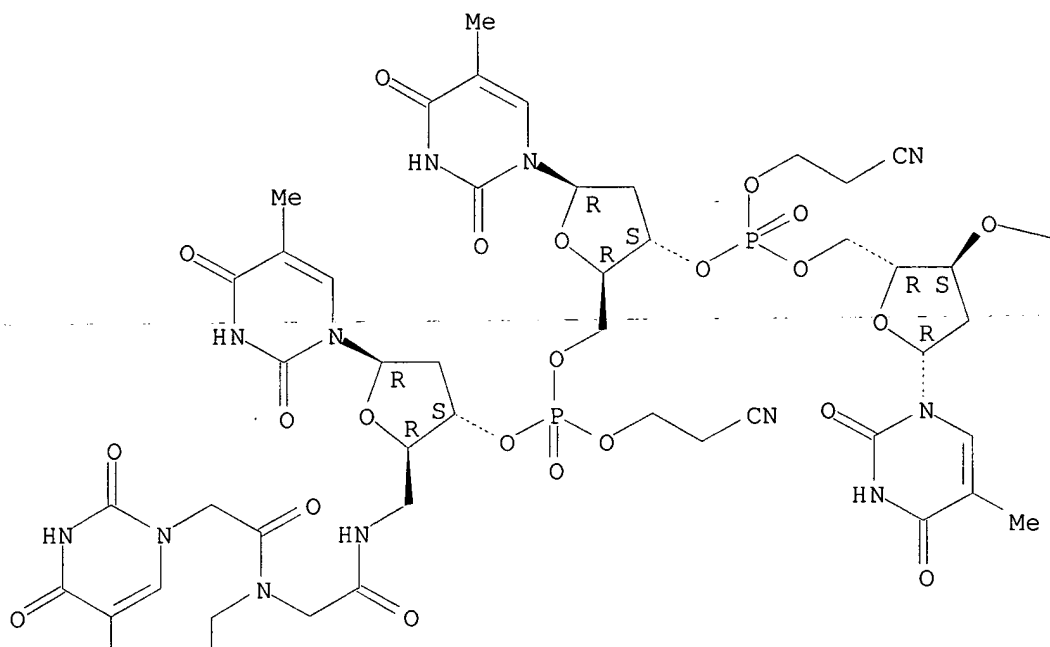
AB The solid support synthesis of a homothymine peptide nucleic acid (PNA)-DNA octamer (i.e. hybrid I; T = thymine-1-yl), which is an antisense oligonucleotide analog (no data), could be realized using tetrabutylammonium N-[2-(4-methoxytrityl)aminoethyl]-N-[(thymine-1-yl)acetyl]glycinate (II) as PNA building block and the resp. 2-cyanoethyl-N,N-diisopropylphosphoramidite derivs. of both 5'-O-(4,4'-dimethoxytrityl)thymidine and 5'-N-(4-methoxytrityl)amino-5'-deoxythymidine (III; R = O-DMTr, NH-MMTr).

IT **170944-01-1DP**, support-bound **170944-02-2DP**, support-bound **170944-03-3DP**, support-bound
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
 (solid support synthesis of homothymine peptide nucleic acid-DNA hybrid as antisense oligonucleotide analog)

RN 170944-01-1 HCAPLUS

CN Thymidine, P-(2-cyanoethyl)-5'-deoxy-5'-[[[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl][2-[[[(4-methoxyphenyl)diphenylmethyl]amino]ethyl]amino]acetyl]amino]thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

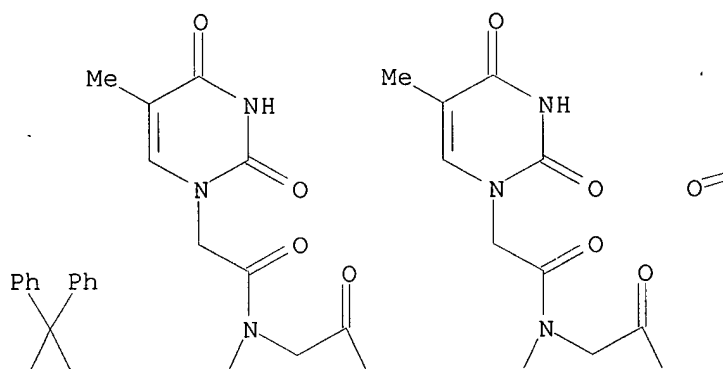


RN 170944-02-2 HCAPLUS

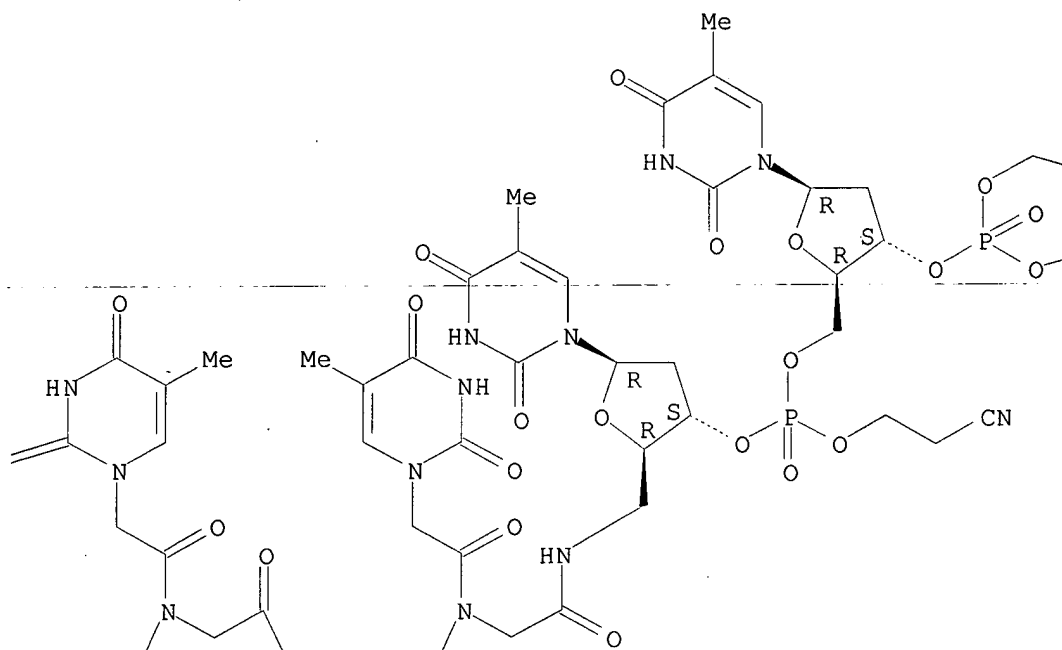
CN Thymidine, P-(2-cyanoethyl)-5'-deoxy-5'-[[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-25-(4-methoxyphenyl)-1,7,13,19-tetraoxo-25,25-diphenyl-3,6,9,12,15,18,21,24-octaazapentacos-1-yl]amino]thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

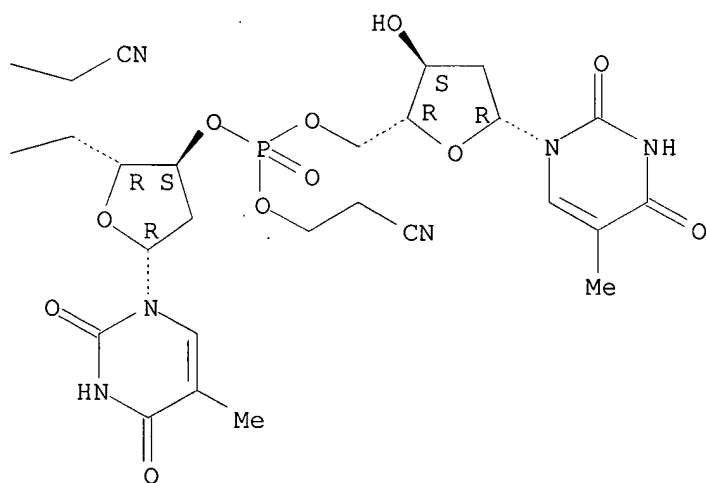
PAGE 1-A

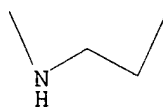
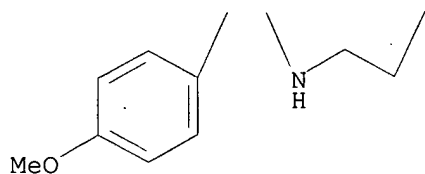


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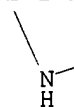


PAGE 1-C

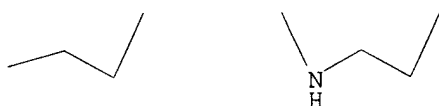




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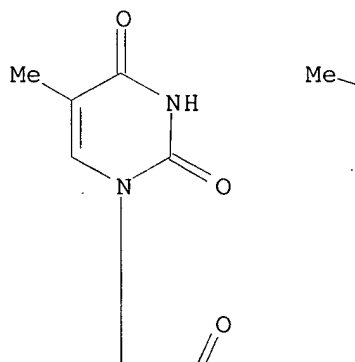
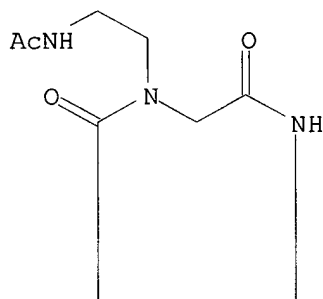


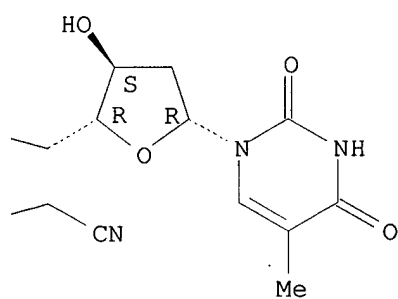
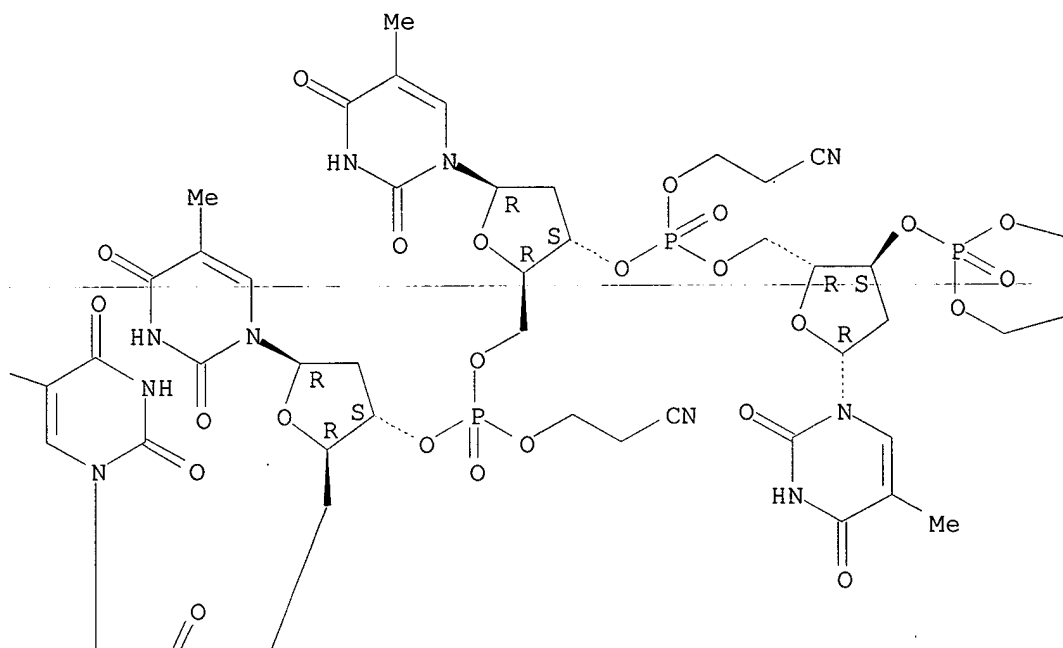
RN 170944-03-3 HCAPLUS

CN Thymidine, P-(2-cyanoethyl)-5'-deoxy-5'-[[[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13,19,25-pentaoxo-3,6,9,12,15,18,21,24-octaazahexacos-1-yl]amino]thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')-P-(2-cyanoethyl)thymidylyl-(3'.fwdarw.5')-(9CI) (CA INDEX NAME)

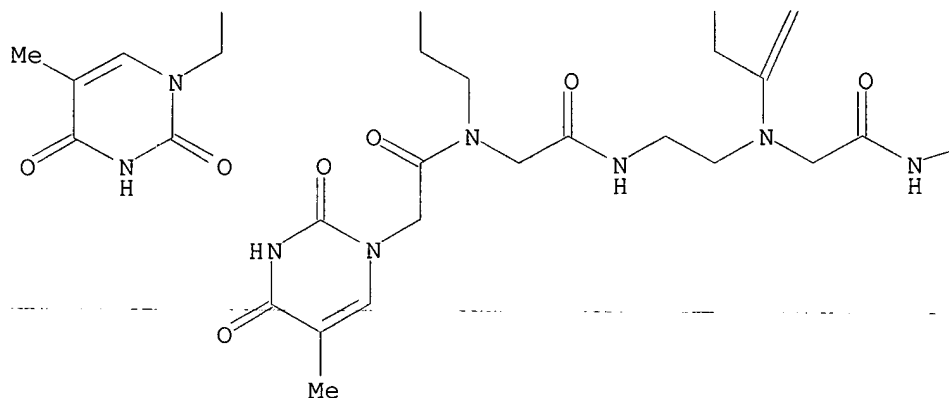
Absolute stereochemistry.

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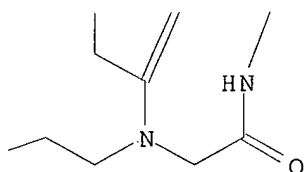




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IT 170944-04-4P

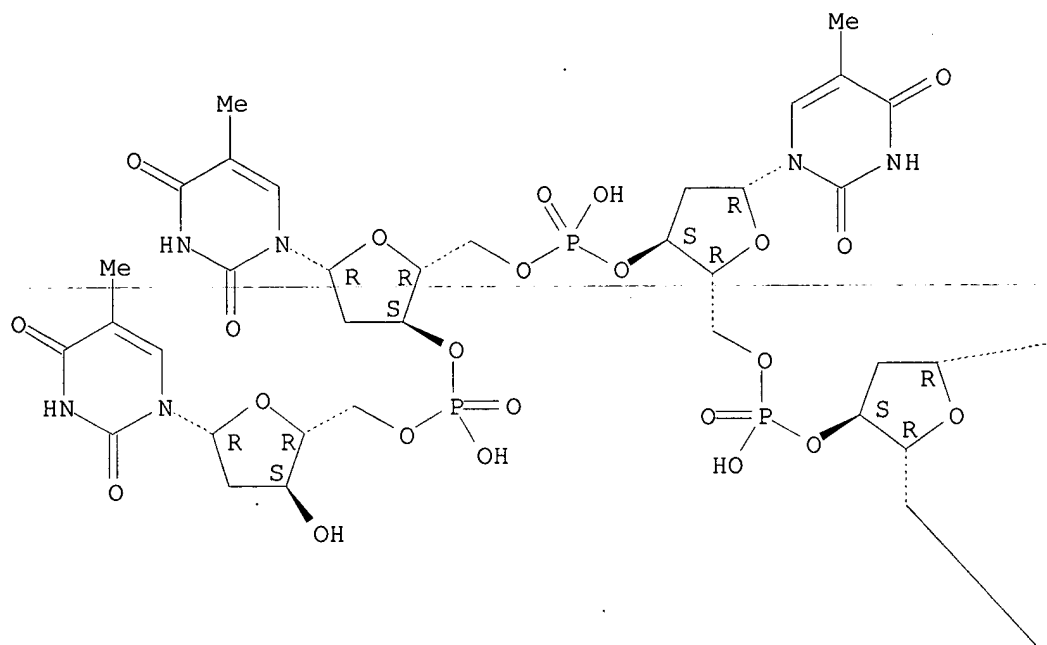
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid support synthesis of homothymine peptide nucleic acid-DNA hybrid
as antisense oligonucleotide analog)

RN 170944-04-4 HCAPLUS

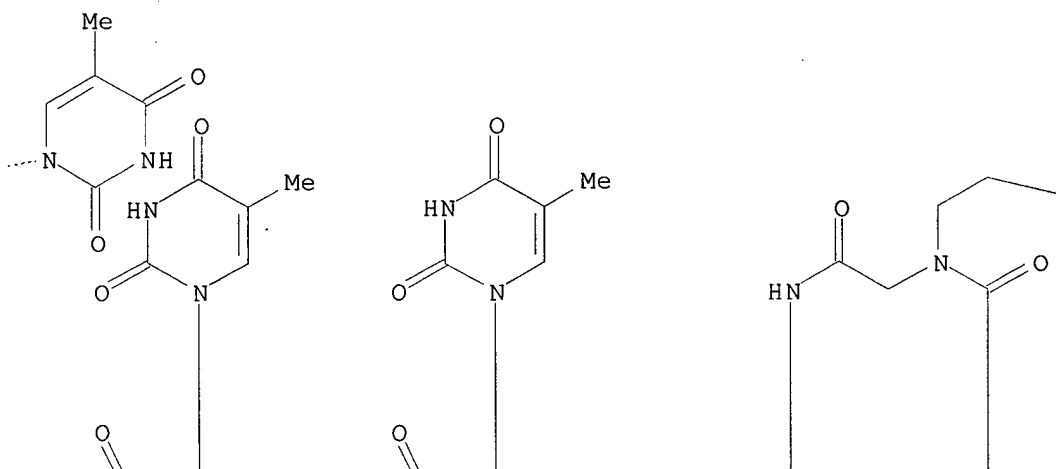
CN Thymidine, 5'-deoxy-5'-[[[3,9,15,21-tetrakis[(3,4-dihydro-5-methyl-2,4-dioxo-1(2H)-pyrimidinyl)acetyl]-1,7,13,19,25-pentaoxo-3,6,9,12,15,18,21,24-octaazahexacos-1-yl]amino]thymidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-thymidylyl-(3'.fwdarw.5')-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

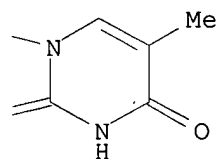
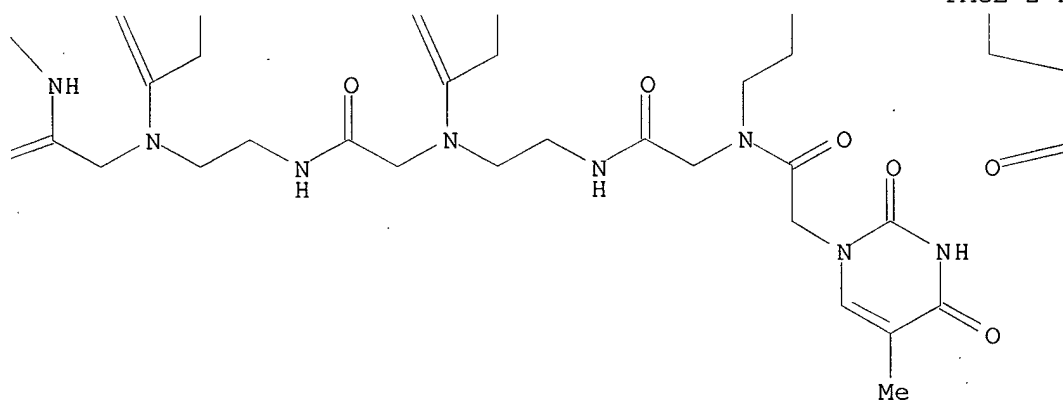
PAGE 1-A



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NHAc



MAUPIN 09/835,371

=> d ibib abs hitstr 14

L13 ANSWER 14 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:435685 HCAPLUS

DOCUMENT NUMBER: 121:35685

TITLE: Synthesis of charged and uncharged complexes of gadolinium and yttrium with cyclic polyazaphosphinic acid ligands for in vivo applications

AUTHOR(S): Pulukkody, Kanthi P.; Norman, Timothy J.; Parker, David; Royle, Louise; Broan, Christopher J.

CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK

SOURCE: J. Chem. Soc., Perkin Trans. 2 (1993), (4), 605-20

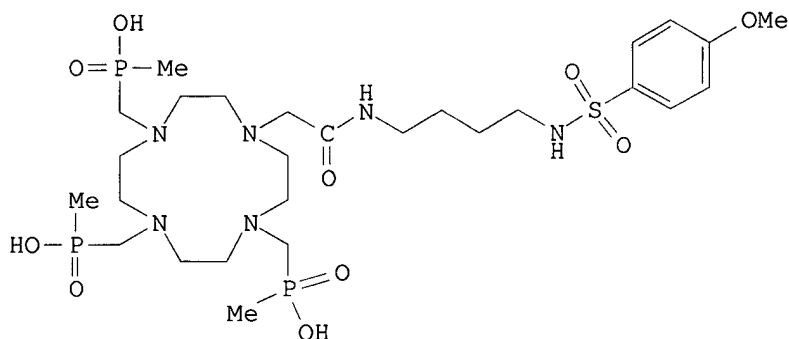
CODEN: JCPKBH; ISSN: 0300-9580

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:35685

GI



I

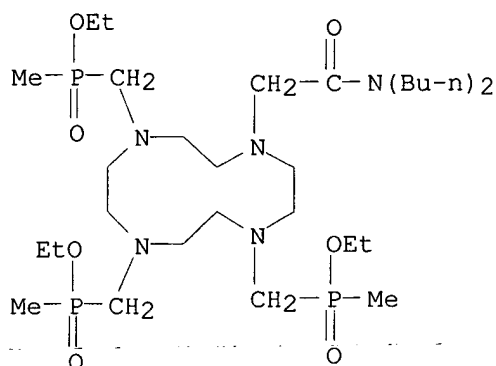
AB The synthesis of 18 new macrocyclic complexing agents incorporating phosphinic acid (and carboxylic acid) groups, e.g., I, is reported, based on the 1,4,7,10-tetraazacyclododecane ring. Through selective functionalization of one ring nitrogen or by changing the nature of the P-substituent, anion, neutral and cationic complexes of yttrium and gadolinium may be prepd. of varying lipophilicity. Diamagnetic complexes have been characterized by ¹H, ³¹P and ⁸⁹Y NMR spectroscopy, and the rate of uptake of ⁹⁰Y of selected ligands compared. The kinetics of dissociation of nine gadolinium complexes has been measured in the pH range 1-2 using ¹⁵³Gd-labeled complexes. Charge-neutral complexes dissociate more slowly than their anionic analogs, and the phosphinate complexes, although slightly less stable than their carboxylate analogs, are nevertheless sufficiently kinetically inert for in vivo applications.

IT 148932-43-8P 148932-55-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and sapon. of)

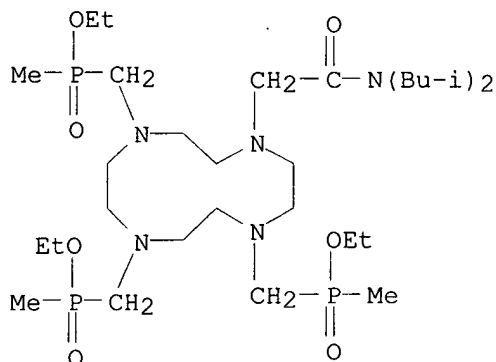
RN 148932-43-8 HCAPLUS

CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl-, triethyl ester (9CI) (CA INDEX NAME)



RN 148932-55-2 HCAPLUS

CN Phosphinic acid, [[10-[2-[bis(2-methylpropyl)amino]-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl-, triethyl ester (9CI) (CA INDEX NAME)

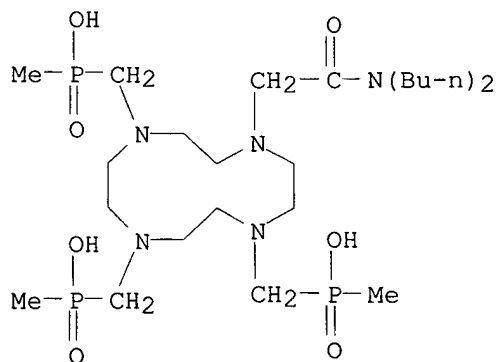


IT 145130-40-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. and uptake with, of yttrium-90)

RN 145130-40-1 HCAPLUS

CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)

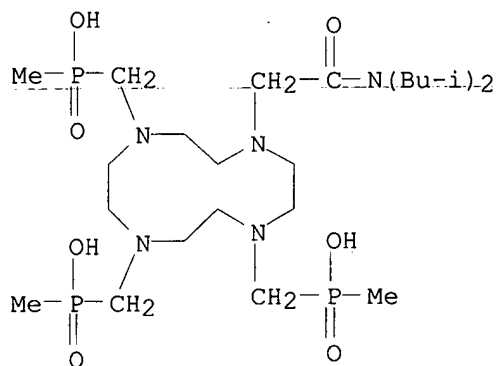


IT 148932-56-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

RN 148932-56-3 HCAPLUS

CN Phosphinic acid, [[10-[2-[bis(2-methylpropyl)amino]-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)



=> d ibib abs hitstr 15

L13 ANSWER 15 OF 15 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:93170 HCAPLUS

DOCUMENT NUMBER: 118:93170

TITLE: Stable anionic, neutral and cationic complexes of gadolinium with functionalized amino-phosphinic acid macrocyclic ligands

AUTHOR(S): Parker, David; Pulukkody, Kanthi; Norman, Timothy J.; Harrison, Alice; Royle, Louise; Walker, Carol

CORPORATE SOURCE: Dep. Chem., Univ. Durham, Durham, DH1 3LE, UK

SOURCE: J. Chem. Soc., Chem. Commun. (1992), (19), 1441-3

CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

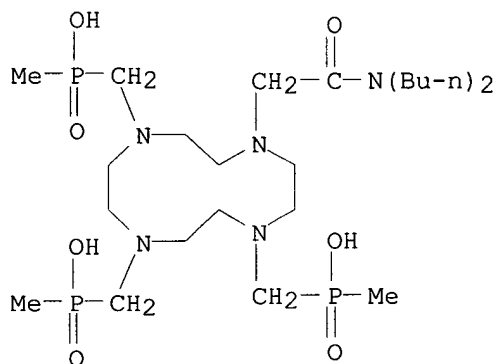
AB The synthesis and stability of anionic, neutral and cationic gadolinium complexes based on tetraazaphosphinic acid ligands is compared: lipophilic anionic complexes show biliary rather than renal clearance. The disson. kinetics was studied.

IT 145130-40-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and acid hydrolysis and deprotection of)

RN 145130-40-1 HCAPLUS

CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)



IT 145130-40-1DP, gadolinium and yttrium complexes

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

RN 145130-40-1 HCAPLUS

CN Phosphinic acid, [[10-[2-(dibutylamino)-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triyl]tris(methylene)]tris[methyl- (9CI) (CA INDEX NAME)

